The one-dimensional Coulomb Problem

G. Abramovici

E-mail: abramovici@lps.u-psud.fr
Laboratoire de Physique des Solides, Univ. Paris Sud, CNRS, UMR 8502, F-91405 Orsay Cedex France

Y. Avishai

E-mail: yshai@bgu.ac.il
Department of Physics and Ilse Katz Center for Nanotechnology, Ben-Gourion University, Beer-Shiva 84105, Israel
Hong Kong University of Science and Technology, Clear Water Bay, Kawloon, Hong Kong

Abstract. One-dimensional scattering by a Coulomb potential $V(x) = \frac{\lambda}{|x|}$ is studied for both repulsive ($c > 0$) and attractive ($c < 0$) cases. Two methods of regularizing the singularity at $x = 0$ are used, yielding the same conclusion, namely, that the transmission vanishes. For an attractive potential ($c < 0$), two groups of bound states are found. The first one consists of *regular* (Rydberg) bound states, respecting standard orthogonality relations. The second set consists of *anomalous* bound states (in a sense to be clarified), which always relax as coherent states.

PACS numbers: 03.65.Ge,03.65.Nk,11.55.Bq,11.55.Ds,73.21.Fg,73.22.Dj

1. Introduction

One-dimensional quantum Hamiltonians are very useful for modeling simple quantum systems. Beside their ubiquitous importance in the study of transmission and tunneling experiments, numerous quantum systems in higher dimensions can be reduced to one-dimensional ones, due to symmetry (for instance radial wave functions in a central potential) or specific physical properties (Josephson junctions or edge states in the quantum Hall effect are just two examples).

The aim of the present work is to examine one-dimensional scattering by a three-dimensional coulomb potential $V(x) = \frac{qq'}{4\pi\epsilon_o|x|}$, starting from the Schrödinger equation with Hamiltonian $H = \frac{p^2}{2m} + V$, for an eigenstate $\psi(x)$, with $x \in \mathbb{R}^* \equiv \mathbb{R} \setminus \{0\}$,

$$-\frac{d^2\psi}{dx^2}(x) + \frac{\lambda}{|x|}\psi(x) = e\psi(x) \ , \tag{1}$$

with $\lambda = \frac{2mqq'}{4\pi\epsilon_o\hbar^2}$ and $e = \frac{2mE}{\hbar^2}$ where E is the energy. $\lambda > 0$ corresponds to the repulsive potential, $\lambda < 0$ to the attractive one; The boundary conditions will be specified later on. This is referred to as the *one-dimensional Coulomb potential problem.* Although it has recently been studied[1], we find it useful to analyze it using somewhat different

approach. As it turns out, there are some subtleties involved, which might affect some of the conclusions reached in Ref. [1].

One of the main advantages encountered in the quantum Coulomb problem is that the exact wave functions are computable. In three dimensions, it has been shown eighty years ago[2] that the asymptotic behavior of the wave functions is somewhat distinct from that of plane waves. This property has been shown to be valid also in one dimension[3].

It proves useful to follow, first, the standard reduction of the Coulomb problem in three dimensions into a radial one-dimensional equation, and to point out the differences between this equation and Eq. (1). Starting from the three-dimensional Schrödinger equation, carrying out partial wave expansion $\Psi(\mathbf{r}) = \sum_{l=0}^{\infty}(2l+1)$ $\psi_l(r)P_l(\cos\theta)$, and writing the radial wave function as $\psi_l(r) = r^{-1}\phi_l(r)$, one obtains the radial Schrödinger equation for $\phi_l(r)$, with $0 < r < \infty$,

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{\lambda}{r}\right]\phi_l(r) = e\phi_l(r) \ . \tag{2}$$

For $l = 0$ (s wave scattering), Eq. (2) has the same form as Eq. (1). The two basic solutions of Eq. (2) are the regular one, satisfying $\phi_l(0) = 0$, and the singular one, satisfying $\phi_l(0) \neq 0$. The singular solution should be discarded: if not, for $l > 0$, the probability of finding the particle in a sphere of radius R, $P_l(R) = \int_0^R \rho_l(r)2\pi r^2 dr$ becomes infinite for any R ; for $l = 0$, the situation is more subtle, $P_0(R)$ remains finite, but the radial current $J_0(R) = \int_0^R j_0(r)2\pi r^2 dr > 0$ becomes nonzero, which is impossible for an s state[4, 5].

A couple of difficulties arise when Eq. (1) is considered as compared with Eq. (2):

(i) The solutions of Eq. (1) are required on $\mathbb{R}^*$, and not only on its positive part $\mathbb{R}^*_+$. Note that H is invariant under space inversion.

(ii) The arguments used in the three-dimensional case to discard singular solutions of Eq. (2) are not valid[6] for the original problem specified by Eq. (1), and the imposition of scattering boundary conditions requires their inclusion as well. The standard techniques used for matching the wave function at $x = 0$ require either the calculation of $\psi'(\varepsilon)$ or of $\int_{-\varepsilon}^{\varepsilon} V(x)dx$ and both quantities diverge logarithmically when $\varepsilon \to 0$. One must then cope with ultraviolet divergences, which need to be regularized.

These difficulties lead us to the *connection problem*, which can be defined as follows: Let us decompose Eq .(1) into two equivalent coupled equations, one defined on $\mathbb{R}^*_+$ with $\tilde{V}(x) = \frac{\lambda}{x}$, the general solutions of which read

$$\psi_+(x) = Af(kx) + Bg(kx) \ , \tag{3a}$$

and the second defined on $\mathbb{R}^*_-$ with $\tilde{V}(x) = -\frac{\lambda}{x}$, the general solutions of which read

$$\psi_-(x) = a\bar{f}(kx) + b\bar{g}(kx) \ . \tag{3b}$$

Here, $f(x{>}0)$ and $\bar{f}(x{<}0)$ are regular solutions, while $g(x{>}0)$ and $\bar{g}(x{<}0)$ are singular solutions, defined on the appropriate domains; the relations between f, g and $\bar{f}, \bar{g}$ will be clarified later on. The connection problem consists in the calculation of the 2×2 matrix expressing (A, B) in terms of (a, b). Since the derivative of the singular solution diverges at $x = 0$, it is impossible to match both ψ and ψ' at $x = 0$. It is also not possible to use the method[7, 8] employed in a problem of scattering by a potential $V(x) = \lambda\delta(x)$ since the latter potential is integrable at $x = 0$, $\int_{-\varepsilon}^{\varepsilon} V(x)dx = \lambda$, whereas

the Coulomb potential is not. Apparently, the connection problem cannot be solved in terms of simple linear relations, and one needs to consider bilinear constraints (an example of such a constraint is the current conservation $J(0^-) = J(O^+)$ around $x = 0$).

Our first task is to properly formulate and solve the scattering problem, corresponding to $e > 0$. To carry it out, we use two independent regularization methods. One is based on bilinear constraints, which can be formulated in such a way that ultraviolet divergences are canceled. The other method consists in calculating the exact transmission for a truncated Coulomb potential V_ε, with $V_\varepsilon(x) = 0$ for $|x| < \varepsilon$, $V_\varepsilon(x) = \lambda/|x|$ for $|x| > \varepsilon$ and letting $\varepsilon \to 0$. With both methods, we arrive at the conclusion that the transmission coefficient vanishes, $T = 0$. The potential is perfectly reflective. Moreover, this property of total reflection also holds for the attractive potential ($\lambda < 0$), whereas classically the reflection vanishes; it is a novel manifestation of perfect *quantum reflection* from an attractive potential. It is distinct from the standard example of quantum reflection from an infinite attractive square well: in the latter case, the divergence of $\int V(x)dx$ is faster than logarithmic, and the corresponding spectrum is not bounded from below.

Our second goal is to calculate bound state energies and wave functions for an attractive potential ($\lambda < 0$) (the one-dimensional "hydrogen atom" problem). The ensuing discrete part of the spectrum ($e < 0$) appears to be rather intriguing, as it is composed of two interlacing spectra. The first one (reported also in Ref. [1, 9]) is the usual Rydberg spectrum, with energies $E_n = -\frac{E_0}{n^2}$, with $n = 1, 2, \ldots$ The corresponding wave functions are the *regular* solutions of the differential Eq. (1). The energies of the second part of the spectrum are shifted from the first ones through $n \to n + 1/2$, that is, $\tilde{E}_n = -\frac{E_0}{(n+\frac{1}{2})^2}$, with $n = 0, 1, \ldots$ The corresponding wave functions will be refereed to as *anomalous* states, and are constructed in terms of the singular solutions of Eq. (1). These solutions are square integrable but not orthogonal. A proper incorporation of such states might require further insight into the basic principles of quantum mechanics.

We organize the rest of the paper as follows: In section 2, we will first study the scattering problem, then explain, in section 3, the two regularization methods used to solve the connection problem. The bound state problem will be analyzed in section 4, where regular and anomalous states are introduced. Finally, a short discussion of our results is carried in section 5. Calculations requiring technical manipulations are collected in the appendices.

2. The scattering problem

2.1. Scattering states

2.1.1. Basic solutions For the scattering problem, we have $e > 0$ in Eq. (1). It is convenient to recast Eq. (1) so that all quantities are dimensionless. Let $k = \sqrt{e}$, $u = kx$, $\eta = \lambda/(2k) = \frac{qq'}{4\pi\epsilon_o\hbar}\sqrt{\frac{m}{2E}}$ and $\varphi(u) = \psi(\frac{u}{k})$. Then the equation for φ is

$$-\frac{d^2\varphi}{du^2}(u) + 2\frac{\eta}{|u|}\varphi(u) = \varphi(u) \ , \quad u \in \mathbb{R}^*, \tag{4}$$

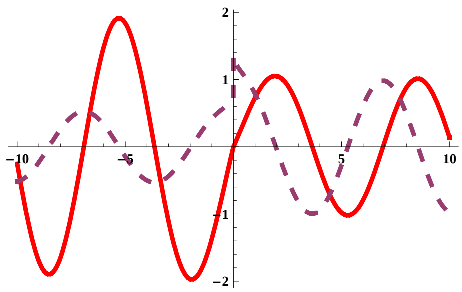

Figure 1. f_η (full line) and g_η (dashed line) for $\eta = 1/5$.

with regular and singular solutions $f_\eta(u)$ and $g_\eta(u)$. Eq. (4) is equivalent to the following couple of equations :

$$-\frac{d^2\varphi}{du^2}(u) + 2\frac{\eta}{u}\varphi(u) = \varphi(u) \quad \text{for } u > 0 \; ; \tag{5a}$$

$$-\frac{d^2\varphi}{du^2}(u) - 2\frac{\eta}{u}\varphi(u) = \varphi(u) \quad \text{for } u < 0 \; . \tag{5b}$$

The solutions of Eq. (5a) are known as Coulomb s wave functions [2, 10] with $L = 0$. We will write $F_\eta(u)$ the regular solution and $G_\eta(u)$ the singular (logarithmic) one:

$$F_\eta(u) = C_\eta u \, \mathrm{e}^{-\mathrm{i}u} M(1 - \mathrm{i}\eta, 2, 2\mathrm{i}u) \; ; \tag{6a}$$

$$\begin{aligned} G_\eta(u) &= \Re\left(2\eta \frac{u\,\mathrm{e}^{-\mathrm{i}u}\Gamma(-\mathrm{i}\eta)}{C_\eta} U(1 - \mathrm{i}\eta, 2, 2\mathrm{i}u)\right) \\ &= 2\eta \frac{u\,\mathrm{e}^{-\mathrm{i}u}\Gamma(-\mathrm{i}\eta)}{C_\eta} U(1 - \mathrm{i}\eta, 2, 2\mathrm{i}u) - \mathrm{i}(-1 + \pi\eta + 2\iota_\eta)F_\eta(u)/C_\eta^2 \; , \end{aligned} \tag{6b}$$

where

$$C_\eta = \mathrm{e}^{-\frac{\pi\eta}{2}} \sqrt{\frac{\pi\eta}{\sinh(\pi\eta)}} \quad \text{and} \quad \iota_\eta = \eta \Im(\Gamma(1 - \mathrm{i}\eta)) \; .$$

In these equations, M is the regular confluent hypergeometric function, also written as ${}_1F_1$, and U is the logarithmic (also called irregular) confluent hypergeometric function[11]. Both F_η and G_η are *real*. Thus, the solutions of Eq. (4) for $u > 0$ are $f_\eta(u) = F_\eta(u)$ and $g_\eta(u) = G_\eta(u)$, $\forall\eta$.

Consider now the domain $u < 0$. In principle, finding the solutions of Eq. (5b) can be achieved by direct continuation of $F_\eta(u)$ and $G_\eta(u)$. Practically, this requires some care, especially for G_η. F_η can be continued analytically since it is regular at $u = 0$, while for $G_\eta(u)$ one has to avoid the divergence of G'_η at $u = 0$. Since (5a) is valid for any sign of η, we simply need to change $\eta \to -\eta$ in the previous expressions, to get the solutions of (5b), thus we get $f_\eta(u) = F_{-\eta}(u)$ and $g_\eta(u) = G_{-\eta}(u)$ $\forall u < 0$ and $\forall\eta$. It should be pointed out that, in the imaginary part of (6b), the factor before F_η does not follow the $\eta \to -\eta$ transformation[12]. The right expression is (note that $C_{-\eta} = \mathrm{e}^{\pi\eta}C_\eta$), $\forall u < 0$:

$$g_\eta(u) = -2\eta \frac{u\,\mathrm{e}^{-\mathrm{i}u}\Gamma(\mathrm{i}\eta)}{C_{-\eta}} U(1 + \mathrm{i}\eta, 2, 2\mathrm{i}u) - \mathrm{i}(-1 + \pi\eta + 2\iota_\eta)F_{-\eta}(u)/C_{-\eta}^2 \; . \tag{6c}$$

One should also note that relations (14.1.14) to (14.1.20) of [10] extend for $\rho < 0$ as soon as one replaces $\log(2\rho)$ by $\log(-2\rho)$ in (14.1.14).

Basic solutions $f_\eta(u)$ and $g_\eta(u)$ are defined on $\mathbb{R}^*$ and shown on Fig. 1. These solutions are constructed so that Eqs. (5a,5b) are satisfied for both $u>0$ and $u<0$, yet the matching condition at $u=0$ is not addressed yet. This will be carried out when we solve the connection problem.

2.1.2. The general solution Having defined the *basic solutions*, we can now form the *general solution* as a linear combination of $f_\eta(u)$ and $g_\eta(u)$, on each side of $u=0$. We use expressions (3a) for $u>0$ and (3b) for $u<0$. Now, the relation between f and $\bar{f}$ and that between g and $\bar{g}$ are well established, so that bar $^-$ can be omitted. With these notations, the general solution writes

$$\varphi(u,\eta)=\begin{cases} Af_\eta(u)+Bg_\eta(u) & \text{for } u>0\ ; \\ af_\eta(u)+bg_\eta(u) & \text{for } u<0\ . \end{cases} \tag{7}$$

The linearity of Schrödinger equation implies that the connection problem eventually reduces in finding the 2×2 matrix D, which obeys

$$\begin{pmatrix} A \\ B \end{pmatrix} = D \begin{pmatrix} a \\ b \end{pmatrix} \qquad \text{with} \qquad \det(D)\neq 0\ . \tag{8}$$

2.1.3. Transfer matrix It should be stressed that D is *not* the transfer matrix $\mathcal{T}$ because $\mathcal{T}$ transforms incoming and outgoing (distorted) plane waves at $u\to-\infty$ to those at $u\to\infty$. In order to identify these asymptotic waves, we need first to examine the asymptotic behavior of the function $\varphi(u,\eta)$ when $u\to\pm\infty$.

The asymptotic behaviors of $F_\eta(u)$ and $G_\eta(u)$, for $u\to+\infty$, have been established a long time ago in Ref. [2]:

$$\begin{aligned} F_\eta(u) &= (1+\frac{\eta}{2u}+\frac{5\eta^2-\eta^4}{8u^2}+..)\sin(u-\Theta_\eta(u))+\ (\frac{\eta^2}{2u}-\frac{2\eta-4\eta^3}{8u^2}+..)\cos(u-\Theta_\eta(u)) \\ &\underset{u\to\infty}{\sim} \sin(u-\Theta_\eta(u))\ ; \end{aligned} \tag{9a}$$

$$\begin{aligned} G_\eta(u) &= (1+\frac{\eta}{2u}+\frac{5\eta^2-\eta^4}{8u^2}+..)\cos(u-\Theta_\eta(u))-\ (\frac{\eta^2}{2u}-\frac{2\eta-4\eta^3}{8u^2}+..)\sin(u-\Theta_\eta(u)) \\ &\underset{u\to\infty}{\sim} \cos(u-\Theta_\eta(u))\ ; \end{aligned} \tag{9b}$$

with

$$\Theta_\eta(u)=\eta\log(2u)-\arg[\Gamma(1+\mathrm{i}\eta)]\ . \tag{10}$$

Derivation of the asymptotic behaviours of $F_\eta(u)$ and $G_\eta(u)$, for $u\to-\infty$, is more subtle. Their determination (6c) and (6d) of Ref. [1] is to be reconsidered[13]. In Appendix A, we find

$$\begin{aligned} F_\eta(u) \ =&\ \ \mathrm{e}^{-\pi\eta}(1+\frac{\eta}{2u}+\frac{5\eta^2-\eta^4}{8u^2}+..)\sin(u-\Theta_\eta(u)) \\ &+\ \mathrm{e}^{-\pi\eta}(\frac{\eta^2}{2u}-\frac{2\eta-4\eta^3}{8u^2}+..)\cos(u-\Theta_\eta(u)) \\ \underset{u\to-\infty}{\sim}&\ \mathrm{e}^{-\pi\eta}\sin(u-\Theta_\eta(u))\ ; \end{aligned} \tag{11a}$$

$$\begin{aligned} G_\eta(u) \ =&\ \ \mathrm{e}^{\pi\eta}(1+\frac{\eta}{2u}+\frac{5\eta^2-\eta^4}{8u^2}+..)\cos(u-\Theta_\eta(u)) \\ &-\ \mathrm{e}^{\pi\eta}(\frac{\eta^2}{2u}-\frac{2\eta-4\eta^3}{8u^2}+..)\sin(u-\Theta_\eta(u)) \\ \underset{u\to-\infty}{\sim}&\ \mathrm{e}^{\pi\eta}\cos(u-\Theta_\eta(u))\ . \end{aligned} \tag{11b}$$

Thus, the asymptotic form of the solution $\varphi(u,\eta)$, is

$$\begin{aligned}\varphi(u,\eta)\underset{u\to\infty}{\widetilde{\quad}}\; & A\sin(u-\Theta_\eta(u))+B\cos(u-\Theta_\eta(u))\\ &= \frac{B-\mathrm{i}A}{2}\,\mathrm{e}^{\mathrm{i}(u-\Theta_\eta(u))}+\frac{B+\mathrm{i}A}{2}\,\mathrm{e}^{\mathrm{i}(\Theta_\eta(u)-u)}\ ; \end{aligned}\tag{12a}$$

$$\begin{aligned}\varphi(u,\eta)\underset{u\to-\infty}{\widetilde{\quad}}\; & a\,\mathrm{e}^{\pi\eta}\sin(u+\Theta_\eta(u))+b\,\mathrm{e}^{-\pi\eta}\cos(u+\Theta_\eta(u))\\ &= \frac{b\,\mathrm{e}^{-\pi\eta}-\mathrm{i}a\,\mathrm{e}^{\pi\eta}}{2}\,\mathrm{e}^{\mathrm{i}(u+\Theta_\eta(u))}+\frac{b\,\mathrm{e}^{-\pi\eta}+\mathrm{i}a\,\mathrm{e}^{\pi\eta}}{2}\,\mathrm{e}^{-\mathrm{i}(\Theta_\eta(u)+u)}\ . \end{aligned}\tag{12b}$$

The transfer matrix $\mathcal{T}$ relates the coefficients of the distorted plane waves at $u\to\infty$ with those at $u\to-\infty$:

$$\begin{pmatrix} B-\mathrm{i}A\\ B+\mathrm{i}A\end{pmatrix}=\mathcal{T}\begin{pmatrix} b\,\mathrm{e}^{-\pi\eta}-\mathrm{i}a\,\mathrm{e}^{\pi\eta}\\ b\,\mathrm{e}^{-\pi\eta}+\mathrm{i}a\,\mathrm{e}^{\pi\eta}\end{pmatrix}. \tag{13}$$

Solution of the scattering problem is equivalent to elucidation of the transfer matrix.

2.2. Scattering

2.2.1. Transmission and reflection amplitudes Alternatively, we define transmission t and reflection r amplitudes in terms of a wave φ_α propagating from $-\infty$ ($\alpha=\mathrm{L}$), or from ∞ ($\alpha=\mathrm{R}$). Explicitly,

$$\varphi_{\mathrm{L}}(u,\eta)\begin{cases}\underset{u\to-\infty}{\widetilde{\quad}} & \mathrm{e}^{\mathrm{i}(u+\Theta_\eta(u))}+r_{\mathrm{L}}\,\mathrm{e}^{-\mathrm{i}(u+\Theta_\eta(u))}\ ;\\[2ex] \underset{u\to\infty}{\widetilde{\quad}} & t_{\mathrm{L}}\,\mathrm{e}^{\mathrm{i}(u-\Theta_\eta(u))}\ ;\end{cases}$$

and

$$\varphi_{\mathrm{R}}(u,\eta)\begin{cases}\underset{u\to\infty}{\widetilde{\quad}} & \mathrm{e}^{-\mathrm{i}(u-\Theta_\eta(u))}+r_{\mathrm{R}}\,\mathrm{e}^{\mathrm{i}(u-\Theta_\eta(u))}\ ;\\[2ex] \underset{u\to-\infty}{\widetilde{\quad}} & t_{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}(u+\Theta_\eta(u))}\ .\end{cases}$$

Time reversal invariance implies $t_{\mathrm{R}}=t_{\mathrm{L}}\equiv t$ and reflection symmetry $H(-x)=H(x)$ implies $r_{\mathrm{R}}=r_{\mathrm{L}}\equiv r$ (to demonstrate it properly, one must note that, if $\varphi(u,\eta)$ is a solution, $\varphi(-u,\eta)$ is another solution, *a priori* independent of the first one). Some useful relations expressing A,B,a,b in terms of t,r are given in Appendix B.

The corresponding transmission and reflection coefficients are

$$T=|t|^2\ ,\quad R=|r|^2\ , \tag{14}$$

and fulfill $R+T=1$ (see Eq. (39a)). For $t\neq 0$, it is instructive to express the ratio of some coefficients a,A in terms of T, once for φ_{L}, and once for φ_{R} (see Appendix B):

$$\begin{aligned}\frac{a_{\mathrm{L}}\,\mathrm{e}^{\pi\eta}}{A_{\mathrm{L}}}&=\epsilon'-2\mathrm{i}\epsilon\sqrt{\frac{1}{T}-1}\ \Rightarrow\ \left|\frac{a_{\mathrm{L}}\,\mathrm{e}^{\pi\eta}}{A_{\mathrm{L}}}\right|=\sqrt{\frac{4}{T}-3}\geq 1\ ;\\ \frac{a_{\mathrm{R}}\,\mathrm{e}^{\pi\eta}}{A_{\mathrm{R}}}&=\frac{1}{\epsilon'-2\mathrm{i}\epsilon\sqrt{\frac{1}{T}-1}}\ \Rightarrow\ \left|\frac{a_{\mathrm{R}}\,\mathrm{e}^{\pi\eta}}{A_{\mathrm{R}}}\right|=\frac{1}{\sqrt{\frac{4}{T}-3}}\leq 1\ ;\end{aligned}$$

these inequalities become equalities only for $T=1$. This proves that the symmetry between the regular and the singular part of a wave function φ which occurs at $x=\pm\infty$ is broken at $x=0$ and that connection relations are not trivial (except for $T=1$ and also the special case $T=0$).

2.2.2. The S matrix The S matrix is related[14, 15] to t and r and writes

$$S = \begin{pmatrix} r & t \\ t & r \end{pmatrix} . \tag{15}$$

Using the unitarity of the S matrix, it is useful to parametrize its elements in terms of the transmission coefficient T and a couple of two independent numbers $\epsilon, \epsilon' = \pm 1$. First, we get the parametrization of all coefficients A_{L}, ..., b_{R}, which we give in Appendix B. Then, we can prove the representation

$$S = \begin{pmatrix} T - 1 + \mathbb{i}\epsilon\epsilon'\sqrt{T - T^2} & \epsilon' T + \mathbb{i}\epsilon\sqrt{T - T^2} \\ \epsilon' T + \mathbb{i}\epsilon\sqrt{T - T^2} & T - 1 + \mathbb{i}\epsilon\epsilon'\sqrt{T - T^2} \end{pmatrix} \tag{16}$$

which is unitary, as required. We stress that this representation is not universal[16], namely, it is peculiar to the Coulomb scattering problem as discussed here.

We are now in a position to examine the connection problem.

3. The connection problem

The connection problem is to relate A, B to a, b either by finding matrix D in Eq. (8), or, equivalently, transfer matrix $\mathcal{T}$ in Eq. (13), or, equivalently, the S matrix in Eq. (15). Since $\frac{\partial \varphi}{\partial u}$ diverges as $u \to 0$, it is not legitimate to use the continuity of φ and $\frac{\partial \varphi}{\partial u}$ at $u = 0$. Thus, the issue of the connection problem can not be handled in solving linear equations of the wave function, and one must address bilinear relations, related either to conservation laws or to certain constraints. In the following analysis, the behaviors of $f_\eta(u)$, $g_\eta(u)$ and of their derivatives, for $u \sim 0$, are required: they are studied in Appendix C.

3.1. Conservation laws and other constraints

3.1.1. Continuity of ρ_η The simplest physical relation that provides a connection at $x = 0$ is the continuity of the density of probability, $\rho_\eta(u) = |\varphi(u, \eta)|^2$. With relations (43a,43b), one gets

$$|B|^2 \, \mathrm{e}^{\pi\eta} = |b|^2 \, \mathrm{e}^{-\pi\eta} \quad \Longleftrightarrow \quad \left| \frac{B}{b} \right| = \mathrm{e}^{-\pi\eta} . \tag{17a}$$

In Appendix B, we show that this relation actually simplifies as

$$B = \epsilon' \, \mathrm{e}^{-\pi\eta} b . \tag{17b}$$

where $\epsilon' = \pm 1$ (note that the case $\epsilon' = -1$ implies a violation of the continuity of ψ).

3.1.2. Current conservation The conservation of current $j(x) = -\Re\Big(\mathbb{i}\overline{\psi(x)}\frac{d\psi}{dx}(x)\Big)$ is equivalent to the unitarity of the S matrix which is already verified. Therefore, it does not help for the resolution of the connection problem.

3.1.3. Orthonormality of scattering states Since the complete set of scattering wave functions is known, it is in principle possible to examine the consequence of generalized orthogonality relations. Let us write $\psi(x, E, \alpha) = \varphi_\alpha(kx, \frac{\lambda}{2k})$ with $\alpha = \mathrm{R}, \mathrm{L}$ (wave functions coming from $+\infty$ or $-\infty$ have degenerate energies),

$$\int dx \, \overline{\psi(x, E_1, \alpha_1)} \psi(x, E_2, \alpha_2) = \delta(k_1 - k_2) P_{\alpha_1 \alpha_2} \tag{18}$$

where P is an unitary 2×2 matrix in the (R,L) space.

In Appendix D, using relations (42a,42b,42c,42d,42e,42f,42g,42h), (12a) and (12b), we calculate[17]

$$\lim_{L\to\infty}\int_{-L}^{L}\overline{\psi(x,E_1,\alpha_1)}\psi(x,E_2,\alpha_2)dx=\Bigg[(1+\frac{\sqrt{R(\eta_2)T(\eta_1)}-\sqrt{R(\eta_1)T(\eta_2)}}{2}\mathcal{Z}\epsilon\epsilon'(1+\mathbb{i}))$$
$$\times\delta(k_1-k_2)+\Bigg(-\frac{R(\eta_1)+R(\eta_2)}{2}+\epsilon\epsilon'\frac{\sqrt{R(\eta_1)T(\eta_1)}+\sqrt{R(\eta_2)T(\eta_2)}}{2}$$
$$+\mathbb{i}(\frac{T(\eta_1)-T(\eta_2)}{2}-\epsilon\epsilon'\frac{\sqrt{R(\eta_1)T(\eta_1)}-\sqrt{R(\eta_2)T(\eta_2)}}{2})\Bigg)\delta(k_1+k_2)+c\Bigg]\delta_{\alpha_1\alpha_2}\ , \quad (19)$$

where c is a constant and $\mathcal{Z}$ a complex number given by,

$$\mathcal{Z}=\sqrt{R(\eta_1)R(\eta_2)}+\sqrt{T(\eta_1)T(\eta_2)}+\mathbb{i}\epsilon\epsilon'(\sqrt{R(\eta_2)T(\eta_1)}-\sqrt{T(\eta_2)R(\eta_1)})\ . \quad (20)$$

Since $k_1,k_2>0$ here, we can drop $\delta(k_1+k_2)$ in Eq. (19), which is irrelevant[18]. The established result in Eq. (19) that $P=I_2$ reflects the orthogonality of left and right moving states. Scattering states can be orthonormalized in the extended sense if and only if $(\sqrt{R(\eta_2)T(\eta_1)}-\sqrt{R(\eta_1)T(\eta_2)})\mathcal{Z}=0$. This yields $T(\eta_1)=T(\eta_2)$ or $T(\eta_i)\in\{0,1\}$. The second condition is actually a particular case of the first one, since otherwise, one could find some energy E such that $T(\eta^+)=1-T(\eta^-)$, which induces a non physical discontinuity; however, this argument will not be needed in the following. Having T independent of E is already a very strong result[16]. Yet, in order to completely elucidate the connection problem, we will now address another constraint.

3.1.4. Hermiticity of the Hamiltonian A successful issue for the connection problem is given by analyzing the hermiticity of Hamiltonian H. For $E_1\neq E_2$, we consider two wave functions $\psi_1: x\mapsto\psi(x,E_1)$ and $\psi_2: x\mapsto\psi(x,E_2)$ (degeneracy is not relevant here, and R,L indices can be omitted). Since H is hermitian, the hermitian product of $|\psi_1\rangle$ with $H|\psi_2\rangle$ must be conjugate with the hermitian product of $|\psi_2\rangle$ with $H|\psi_1\rangle$. Explicitly,

$$\int dx\overline{\psi(x,E_1)}\left[-\frac{\partial^2\psi}{\partial x^2}(x,E_2)+\frac{\lambda}{|x|}\psi(x,E_2)\right]=\int dx\left[-\overline{\frac{\partial^2\psi}{\partial x^2}(x,E_1)}+\frac{\lambda}{|x|}\overline{\psi(x,E_1)}\right]\psi(x,E_2)$$
$$\iff\int dx\ \overline{\psi(x,E_1)}\frac{\partial^2\psi}{\partial x^2}(x,E_2)-\overline{\frac{\partial^2\psi}{\partial x^2}(x,E_1)}\psi(x,E_2)=0\ ,$$

so that

$$\left[-\overline{\psi(x,E_1)}\frac{\partial\psi}{\partial x}(x,E_2)+\overline{\frac{\partial\psi}{\partial x}(x,E_1)}\psi(x,E_2)\right]_{-\infty}^{\infty}=0\ . \quad (21)$$

In Eq. (21), we calculate the Cauchy principal value of the left term, which writes, in terms of dimensionless variables and function φ :

$$\lim_{L\to\infty}\frac{\lambda}{2}\left[-\frac{\overline{\varphi(u,\eta_1)}}{\eta_2}\frac{\partial\varphi}{\partial u}(u,\eta_2)+\overline{\frac{\partial\varphi}{\partial u}(u,\eta_1)}\frac{\varphi(u,\eta_2)}{\eta_1}\right]_{-L}^{L}. \quad (22a)$$

Since $-\overline{\varphi(u,\eta_1)}\frac{\partial\varphi}{\partial u}(u,\eta_2)+\overline{\frac{\partial\varphi}{\partial u}(u,\eta_1)}\varphi(u,\eta_2)$ is divergent at $u=0$, one must use regularized integral around zero. Hence one should add the Cauchy principal value:

$$\lim_{\varepsilon\to 0^+}\frac{\lambda}{2}\left[\frac{\overline{\varphi(u,\eta_1)}}{\eta_2}\frac{\partial\varphi}{\partial u}(u,\eta_2)-\overline{\frac{\partial\varphi}{\partial u}(u,\eta_1)}\frac{\varphi(u,\eta_2)}{\eta_1}\right]_{-\varepsilon}^{\varepsilon} \tag{22b}$$

and Eq. (21) writes (22a)+(22b)=0. The contribution (22a) is found to vanish when $L\to\infty$ (detailed calculations, using relations (12a), (42e, 42f, 42g, 42h), are given in Appendix E) so the net expression of Eq. (21) is determined by (22b) which yields

$$\begin{aligned}0=\mathcal{Z}\Big\{&\epsilon\epsilon'\big(\frac{C_{\eta_1}}{\eta_1 C_{\eta_2}}\sqrt{R(\eta_1)T(\eta_2)}-\frac{C_{\eta_2}}{\eta_2 C_{\eta_1}}\sqrt{T(\eta_1)R(\eta_2)}\big)\\&+\frac{2}{C_{\eta_1}C_{\eta_2}}\Re\Big(\Gamma(1+\mathbb{i}\eta_2)-\Gamma(1+\mathbb{i}\eta_1)\Big)\sqrt{T(\eta_1)T(\eta_2)}\Big\}\ .\end{aligned}$$

Employing relations (42a,42b,42c,42d), we get the very same equation. Note that $h_1(\eta_1,\eta_2)\equiv\frac{C_{\eta_1}}{C_{\eta_2}}$, $h_2(\eta_1,\eta_2)\equiv\frac{C_{\eta_2}}{C_{\eta_1}}$ and $h_3(\eta_1,\eta_2)\equiv\frac{1}{C_{\eta_1}C_{\eta_2}}$ are independent two-variable functions. Indeed, let us assume a linear combination,

$$\gamma_1 h_1+\gamma_2 h_2+\gamma_3 h_3=0. \tag{23}$$

Since $\sqrt{\frac{x}{\sinh(x)}}$ and $\sqrt{\frac{\sinh(x)}{x}}$ are one-variable independent functions, if one keeps η_2 constant and considers Eq. (23) as an equation of variable η_1, one gets $\gamma_1=0$; if one keeps η_1 constant and considers Eq. (23) as an equation of variable η_2, one gets $\gamma_2=0$; thus, $\gamma_3=0$ and the independence of the three functions is proved. Now $\mathcal{Z}$, defined in (20), can never vanish. Hence one gets

$$R(\eta_1)T(\eta_2)=0\ ;\ T(\eta_1)R(\eta_2)=0\ ;\ T(\eta_1)T(\eta_2)=0\ .$$

The first two equations imply $T=0,1$, and the last one simply implies $T=0$. This eventually proves[16] that, indeed, $T(\eta)=0$.

3.2. Regularization by truncation of the potential

Here we propose another approach, which gives the same result: the divergences are regularized by a truncation of the potential.

3.2.1. Truncated half-potential In order to avoid the use of Coulomb wave functions for negative argument we calculate transmission and reflection amplitudes for a right half-barrier, defined for $x>0$, and then use reflection symmetry to calculate them for a mirror symmetric barrier, defined for $x<0$. Then left and right barriers are combined using a composition formula for the S matrix, as suggested for instance in Ref. [19].

The truncated right half-potential is, see Fig. 2,

$$V_\varepsilon(x)=\begin{cases}0 & \text{for } x\le\varepsilon\ ;\\ \dfrac{\lambda}{x} & \text{for } x>\varepsilon\ .\end{cases} \tag{24}$$

and the Schrödinger equation with $V_\varepsilon(x)$ alone writes $-\frac{d^2\psi(x)}{dx^2}+V_\varepsilon(x)\psi(x)=k^2\psi(x)$.

In order to avoid the $1/|x|$ singularity, the potential is assumed to be zero for $0<x<\varepsilon$, but we have also performed our calculations with $V_\varepsilon(x{<}\varepsilon)=\frac{\lambda}{\varepsilon}$, with no

significant changes. The cutoff parameter $\varepsilon > 0$ is assumed small, and eventually the limit $\varepsilon \to 0$ is taken on the sum of left and right barriers, which corresponds to the complete Coulomb potential, since

$$\frac{2m}{\hbar^2} V(x) = \lim_{\varepsilon \to 0} V_\varepsilon(x) + V_\varepsilon(-x) \ . \tag{25}$$

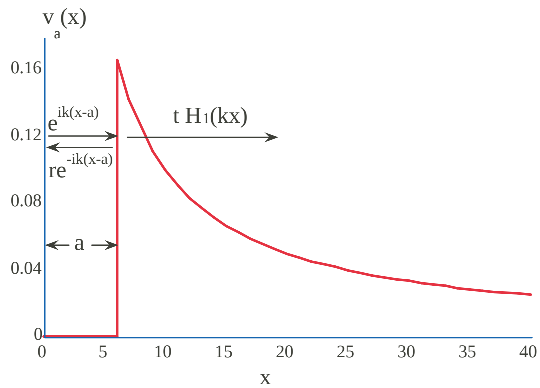

Figure 2. Right-half truncated potential (24) and wave function in the two regions following Eq. (26).

To calculate transmission and reflection amplitudes for the right barrier consider a plane wave approaching the potential V_ε from $-\infty$. It is partially reflected by the barrier at $x = \varepsilon$, and the transmitted wave is a Coulomb wave $tH\eta$, with $H_\eta(u) = F_\eta(u) + \mathbb{i} G_\eta(u)$. Its asymptotic behavior is

$$H_\eta(u) \underset{u \to \infty}{\sim} \mathrm{e}^{\mathbf{i}(u - \Theta_\eta(u))} \ .$$

The scattering boundary conditions for the wave function are, see figure 2,

$$\psi(x) = \begin{cases} e^{\mathbf{i}k(x-\varepsilon)} + r e^{-\mathbf{i}k(x-\varepsilon)} & \text{for } x \le \varepsilon \ , \\ t H_\eta(kx) & \text{for } x > \varepsilon \ . \end{cases} \tag{26}$$

We want to calculate reflection and transmission amplitudes r and t for this right-half truncated Coulomb barrier $V_\varepsilon(x)$. Matching at $x = \varepsilon$ yields

$$1 + r = t H_\eta(k\varepsilon) \ , \quad 1 - r = -\mathbb{i} t \dot{H}_\eta(k\varepsilon) \ ,$$

where $\dot{H}$ stands for dH/du, and thus

$$t = \frac{2}{H_\eta(k\varepsilon) - \mathbb{i}\dot{H}_\eta(k\varepsilon)} \ ; \quad r = \frac{H_\eta(k\varepsilon) + \mathbb{i}\dot{H}_\eta(k\varepsilon)}{H_\eta(k\varepsilon) - \mathbb{i}\dot{H}_\eta(k\varepsilon)} \ . \tag{27}$$

In the limit $\varepsilon \to 0$, this implies

$$t \to 0 \ , \quad r \to -1 \ .$$

However, the limit $\varepsilon \to 0$ will not be taken here, but rather, at a later step.

So far, we have considered transmission and reflection from the potential $V_\varepsilon(x)$ where the incoming wave approaches the barrier from the left region. If the wave would have come from the right, be partially transmitted to the left and partially

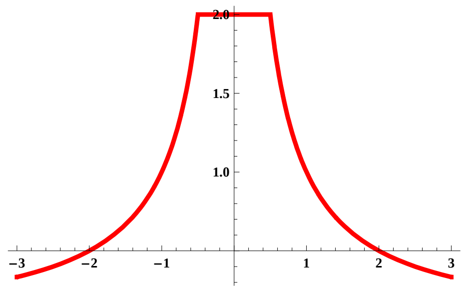

Figure 3. Truncated potential for $\eta = 1$, $\lambda = 1$ and $\varepsilon = 1$.

reflected back to the right, the transmission amplitude would be the same, but the reflection would have a different phase. However,when we combine the symmetric image of $V_\varepsilon(x)$ in order to account for the Coulomb problem as asserted in Eq. (25), we employ the reflection amplitude r, as a result of the analysis developed in Ref. [19]. This procedure of combining the two barriers should be used *before* the limit $\varepsilon \to 0$ is taken on Eqs. (27). The transmission amplitude through the combined barrier $V_\varepsilon(x) + V_\varepsilon(-x)$ is

$$\begin{aligned} T_\varepsilon &= \frac{t^2}{1 - e^{2\mathbb{i}k\varepsilon} r^2} \\ &= \frac{4}{(1 - e^{2\mathbb{i}k\varepsilon})[H_\eta(k\varepsilon)^2 - \dot{H}_\eta(k\varepsilon)^2)] - 2\mathbb{i}(1 + e^{2\mathbb{i}k\varepsilon}) H_\eta(k\varepsilon)\dot{H}_\eta(k\varepsilon)} . \end{aligned} \tag{28}$$

This formula is exact and expresses the transmission amplitude for a symmetric combination of cutoff Coulomb barriers with a hole between $-\varepsilon$ and ε. It uses Coulomb wave functions solely with positive argument. Inspecting the two terms of the denominator in Eq. (28), the first term is found to vanish in the limit $\varepsilon \to 0$, and hence:

$$T_\varepsilon \approx \frac{\mathbb{i}}{H_\eta(k\varepsilon)\dot{H}_\eta(k\varepsilon)} \underset{\varepsilon\to 0}{\longrightarrow} 0 .$$

The upshot is that the transmission coefficient of combined left and right barriers, which comprise Coulomb barrier as $\varepsilon \to 0$, vanishes, that is $T = \lim_{\varepsilon\to 0} T_\varepsilon = 0$.

3.2.2. A second form of truncated potential We also considered a truncated potential V_ε, represented in Fig. 3 and defined as follow: $\varepsilon > 0$ and $\forall |x| \le \varepsilon$, $V_\varepsilon(x) = \frac{\lambda}{\varepsilon}$, $\forall |x| > \varepsilon$, $V_\varepsilon(x) = \frac{\lambda}{|x|}$.

The transmission T_ε can again be exactly calculated (the wave function ψ corresponding to given (E, ε) and its derivative ψ' are continuous; we use first order Taylor expansion for the Coulomb wave functions at connection points $x = \pm\varepsilon$).

One finds, in Fig. 4 the curves of T_ε versus ε, for repulsive or attractive cases. We see that the transmission $T_\varepsilon \to 0$ as $\varepsilon \to 0$. This confirms our analytical result. We must precise that for some points of these figures, we used about 1000 digit precision calculation, provided by a formal calculation with integers.

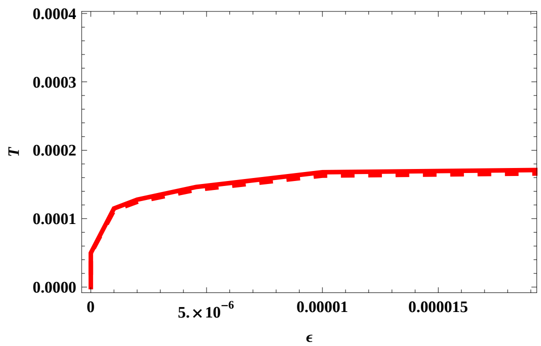

Figure 4. Transmission T_ε versus ε in the repulsive (plain line) or attractive (dashed line) case.

4. Discrete spectrum : bound states

We come now to the case of an attractive potential, and look for bound states of negative energies. As is shown below, analytical expressions can be obtained for the energies as well as for the wave functions[20].

4.1. Analytical solutions

For $e < 0$, Eq. (4) is modified so that its right term writes $-\varphi(u)$ instead of $\varphi(u)$. Note that $u = kx$ holds but now $k = \sqrt{-e}$, since, for an attractive potential, $\eta < 0$. We will again consider separately $u > 0$ and $u < 0$, and hence get the corresponding two equations:

$$-\frac{d^2\varphi}{du^2}(u) + 2\frac{\eta}{u}\varphi(u) = -\varphi(u) \quad \text{for } u > 0 \; ; \tag{29a}$$

$$-\frac{d^2\varphi}{du^2}(u) - 2\frac{\eta}{u}\varphi(u) = -\varphi(u) \quad \text{for } u < 0 \; . \tag{29b}$$

In order to solve Eq. (29a), we need to generalize equations (14.1.6), (14.1.14), (14.1.18), (14.1.19) and (14.1.20) of Ref. [10] (for $L = 0$). This is carried out in Appendix G. Generalization of (14.1.3) in Ref. [10] is given below; relations (14.1.4), (14.1.5), (14.1.15), (14.1.17) remain valid by construction. Incidentally, the results of Appendix G can be regarded as a hyperbolic version of the original relations in Ref. [10], since the solutions of Eq. (29a) now read:

$$J_\eta(u) \equiv u\,\mathrm{e}^{-u} M(1+\eta, 2, 2u)\;, \qquad K_\eta(u) \equiv 2u\,\mathrm{e}^{-u} U(1+\eta, 2, 2u)\;.$$

In analogy with the case of free states, the functions $J_{-\eta}$ and $K_{-\eta}$ are solutions of (29b) (the connection problem at $u = 0$ will be elucidated later on). A useful identity, which will be needed, is

$$J_{-\eta}(u) = -J_\eta(-u)\;. \tag{30}$$

4.2. Quantization

For an arbitrary value of η, the solutions $J_\eta(u)$ and $K_\eta(u)$ of Eq. (29a) diverge as $u \to \infty$ and the solutions $J_{-\eta}(u)$ and $K_{-\eta}(u)$ of Eq. (29b) diverge as $u \to -\infty$. This

is true for almost all values of η, which therefore should be discarded as non physical, except for a set of quantized values η_n (equivalently e_n or E_n) such that $J_\eta(u > 0)$ and $J_{-\eta}(u < 0)$ are both square integrable, and for another set of values $\tilde{\eta}_n$ (equivalently $\tilde{e}_n$ or $\tilde{E}_n$) such that $K_\eta(u > 0)$ and $K_{-\eta}(u < 0)$ are both square integrable. The complete spectrum, which is described below, is composed of the union of set $\{E_n\}$, which is exactly Rydberg's spectrum, and set $\{\tilde{E}_n\}$, the existence of which is indeed a surprise.

4.2.1. The regular solutions Following the analysis of the hydrogen like atoms, it is verified that regular solutions $J_\eta(u)$ and $J_{-\eta}(u)$ decay exponentially as $u \to \pm\infty$ only for a discrete set $\{\eta_n, \forall n \in \mathbb{N}^\star\}$ given by

$$\eta = \eta_n \equiv -n \quad \Longleftrightarrow \quad E = E_n \equiv -\frac{(qq')^2 m}{2(4\pi\epsilon_o)^2\hbar^2 n^2} \; . \tag{31}$$

The corresponding energies E_n form the Rydberg spectrum of hydrogen like atoms. In particular, the lowest energy is $E_1 = -\frac{(qq')^2 m}{2(4\pi\epsilon_o)^2\hbar^2} = -ZZ'E_I$, where E_I is the Rydberg energy.

The question whether the set η_n defined above can be used also for the singular solutions is answered negatively, although the demonstration is not immediate. While $K_{-\eta_n}(u)$ diverges as $u \to -\infty$, $K_{\eta_n}(u)$ *does not diverge* as $u \to \infty$. Therefore, one may consider a mixed solution $AJ_{\eta_n} + BK_{\eta_n}$ for $u > 0$ and $aJ_{-\eta_n}$ for $u < 0$. However, as we shall see immediately below, $J_{\eta_n}(0) = J_{-\eta_n}(0) = 0$, while $K_{-n}(0^+) = 1/C_{-\eta_n}$. Hence the continuity of the density ρ at $x = 0$ implies here $|B| = 0$, which proves that a combination of regular and singular solutions is not an eigenstate.

So far we have asserted the exponential decay of $J_{\pm\eta_n}$ as $u \to \pm\infty$. The complete regular solutions $\forall n \in \mathbb{N}^*$ can be constructed as $\zeta_n(u) = J_{\eta_n}(u)\ \forall u > 0$ and $\zeta_n(u) = -\mu J_{\eta_n}(-u)\ \forall u < 0$, with $\mu \in \mathbb{C}$, (due to Eq. (30) and the reflection symmetry between Eqs. (29a) and (29b)). Explicitly (cf. Eq. (13.6.9) of Ref. [10]),

$$\zeta_n(u) = -\frac{u}{n}\,\mathrm{e}^{-|u|}L'_n(2|u|)\begin{cases} 1 & \text{for } u > 0 \;, \\ \mu & \text{for } u < 0 \;, \end{cases} \tag{32}$$

where $L_n(z)$ is the Laguerre polynomial of order n, and $L'_n(z) = \frac{dL_n(z)}{dz}$. It will be shown below that $\mu = \pm 1$.

The orthogonality and normalization of the corresponding wave functions $\psi(x, E_n) = \zeta_n(\frac{\lambda x}{2\eta_n}) = \zeta_n(\frac{|\lambda| x}{2n})$ can be inspected by carrying out integration on the positive semi axis $\mathbb{R}_+$. Thus, for the normalization we have,

$$\int_0^\infty dx\ |\psi(x, E_n)|^2 = \int_0^\infty dx\ |\zeta_n(kx)|^2 = \frac{1}{k}\int_0^\infty du\ |\zeta_n(u)|^2 = \frac{2n}{|\lambda|}\frac{n}{4} = \frac{n^2}{2|\lambda|} \; ;$$

which, with $|\mu| = 1$, requires a normalization factor equal to $\frac{\sqrt{|\lambda|}}{n}$; while for the orthogonality we find,

$$\int_0^\infty dx\ \overline{\psi(x, E_n)}\psi(x, E_{n'}) = \int_0^\infty dx\ \overline{\zeta_n(\frac{|\lambda| x}{2n})}\zeta_{n'}(\frac{|\lambda| x}{2n'}) = 0 \quad \forall n \neq n' \; ,$$

due to orthogonality relations between Laguerre polynomials.

4.2.2. Anomalous solutions Quite remarkably, the anomalous solutions $K_\eta(u)$ and $K_{-\eta}(u)$ both decay exponentially as $u \to \pm\infty$ only for a discrete set $\{\tilde{\eta}_n, \forall n \in \mathbb{N}\}$ given by

$$\eta = \tilde{\eta}_n = -n - \frac{1}{2} \iff E = \tilde{E}_n \equiv E_{n+\frac{1}{2}} = -\frac{(qq')^2 m}{2(4\pi\epsilon_o)^2\hbar^2(n+\frac{1}{2})^2}\ , \tag{33}$$

where E_n is that of Eq. (31). The corresponding energies $\tilde{E}_n$ form a separate spectrum interlacing the Rydberg one. From Eq. (33), one notes that $\tilde{E}_n = \frac{p^2}{(n+\frac{1}{2})^2}E_p$, $\forall p \in \mathbb{N}^*$, so that the minimum $\tilde{E}_0$ is lower than E_1 by a factor of 4.

Note that, for $\eta \neq \tilde{\eta}_n$, $K_{-\eta}(u)$ is diverging exponentially for $u \to -\infty$, while $K_\eta(u)$ does not diverge for $u \to \infty$. Therefore, one should examine the possibility of a continuous spectrum, by constructing a solution $AK_\eta(u)$ for $u > 0$ and zero for $u < 0$ for any such $\eta \neq \tilde{\eta}_n$; however, one can calculate $K_\eta(0^+) = 1/C_\eta \neq 0$ for all $\eta < 0$, so the continuity of the density ρ at $x = 0$ implies $A = 0$. This possibility is eventually discarded.

So far we have asserted the exponential decay of $K_{\pm\tilde{\eta}_n}$ as $u \to \pm\infty$. In order to construct the complete anomalous solutions, one needs to examine first the properties of $K_{-\tilde{\eta}_n}(u)$ for $u < 0$ and $n \in \mathbb{N}$. The imaginary part writes

$$\Im(K_{-\tilde{\eta}_n}(u)) = \frac{\sqrt{\pi}}{\gamma_n} J_{\tilde{\eta}_n}(u) \qquad \text{with} \quad \gamma_n = (2n-1)!!/2^{n+1}\ ;$$

while, for the real part, there is a relation analogous to (30) :

$$K_{\tilde{\eta}_n}(-u) - \mathbb{i}\frac{\sqrt{\pi}}{\gamma_n} J_{\tilde{\eta}_n}(-u) = \nu_n K_{-\tilde{\eta}_n}(u) \qquad \forall u > 0 \tag{34}$$

where $\nu_n = 2^{2n+1}/((2n+1)(2n-1)!!)^2)$: $K_{\tilde{\eta}_n}$ has even parity (whereas J_{η_n} has odd parity) if one omits rescaling factor ν_n.

The complete anomalous solutions $\forall n \in \mathbb{N}$ can then be defined as $\xi_n(u) = K_{\tilde{\eta}_n}(u)$ for $u > 0$ and $\xi_n(u) = \nu K_{\tilde{\eta}_n}(-u)$ for $u < 0$, due to Eq. (34) and the reflection symmetry between Eqs. (29a) and (29b). It is not necessary to include the factor ν_n here, since it is accounted for by the coefficient ν. The latter will be shown below to be $\nu = \pm 1$. In Appendix H, we prove that the anomalous solutions are explicitly given by

$$\xi_n(u) = (p_n(|u|)\mathbf{K}_0(|u|) + q_n(|u|)\mathbf{K}_1(|u|))\frac{|u|}{(-2)^n\sqrt{\pi}} \times \begin{cases} 1 & \text{for } u > 0\ , \\ \nu & \text{for } u < 0\ , \end{cases} \tag{35}$$

where polynomials $p_n(x)$ and $q_n(x)$ follow recurrence Eqs. (47a) and (47b), and $\mathbf{K_n}$ are the Bessel functions of the second kind. For instance, $p_0 = q_0 = 1$, $p_1(x) = 3 - 4x$, $q_1(x) = 1 - 4x$, $p_2(x) = 4x(4x - 9) + 15$ and $p_2(x) = 4x(4x - 7) + 3$ (more generally, these polynomials are proved to be real with integer coefficients in Appendix H). We are unaware of any occurrence of this family of polynomials, which are worth being studied further.

As for determining the constant ν, contrary to the regular case, $\xi_n(0) \neq 0$. Hence, from the continuity of the density ρ, we deduce that

$$\left|\xi_n(0^-)\right| = \left|\xi_n(0^+)\right|$$

in analogy with Eq. (17a). This implies $\nu = \pm 1$ (we are studying real solutions). Thus, the anomalous solution ξ_n is even for $\nu = 1$ and odd for $\nu = -1$.

Similarly to the case of regular solutions, the orthogonality and normalization of the corresponding wave functions $\psi(x,\tilde{E}_n)=\xi_n(\frac{\lambda x}{2\tilde{\eta}_n})=\xi_n(\frac{|\lambda|x}{2n+1})$ can be inspected by carrying out integration on the positive semi axis $\mathbb{R}_+$. Thus, for the normalization we have,

$$\int_0^\infty dx|\psi(x,\tilde{E}_n)|^2=\int_0^\infty dx|\xi_n(kx)|^2=\frac{1}{k}\int_0^\infty du|\xi_n(u)|^2=\frac{1}{|\lambda|}\left(\frac{(2n+1)\beta_n}{2^{2n+2}\pi}+\frac{\nu_n\pi}{2^{n+3}}\right)$$

The first coefficients β_n can be easily computed, $\beta_0=3$, $\beta_1=41$, $\beta_2=1063$. For large n, $\beta_n\sim 5(2n+1)!!$. Since we proved $\nu=\pm1$, one can deduce the exact normalization factor.

Strikingly, the anomalous solutions are not orthogonal to each other. As a counter example, consider three hermitian products between anomalous states ξ_n and ξ_p with $(n,p)=(0,1)$, $(0,2)$ and $(1,2)$, on the semi-axis $\mathbb{R}_+$:

$$\begin{aligned}\int_0^\infty dx\overline{\psi(x,\tilde{E}_0)}\psi(x,\tilde{E}_1) &= \int_0^\infty dx\overline{\xi_0(|\lambda|x)}\xi_1(\frac{|\lambda|x}{3})\\ &= \frac{2}{|\lambda|}(\frac{3}{8\pi}-\frac{9(\mathsf{E}(-8)-3\mathsf{E}(\frac{8}{9})-3\mathsf{K}(-8)+\mathsf{K}(\frac{8}{9}))+3\ln(729)}{64})\\ &\simeq \frac{2}{|\lambda|}0.0210133\end{aligned}$$

$$\begin{aligned}\int_0^\infty dx\overline{\psi(x,\tilde{E}_0)}\psi(x,\tilde{E}_2) &= \int_0^\infty dx\overline{\xi_0(|\lambda|x)}\xi_2(\frac{|\lambda|x}{5})\\ &= \frac{2}{|\lambda|}(-\frac{35}{48\pi}+\frac{175(\mathsf{E}(-24)-5\mathsf{E}(\frac{24}{25})-4\mathsf{K}(-24)+\frac{4}{5}\mathsf{K}(\frac{24}{25}))+27\ln(5)}{1728})\\ &\simeq -\frac{2}{|\lambda|}0.0319898\end{aligned}$$

$$\begin{aligned}\int_0^\infty dx\overline{\psi(x,\tilde{E}_1)}\psi(x,\tilde{E}_2) &= \int_0^\infty dx\overline{\xi_1(\frac{|\lambda|x}{3})}\xi_2(\frac{|\lambda|x}{5})\\ &= \frac{2}{|\lambda|}(\frac{45}{32\pi}-\frac{45(2705(3\mathsf{E}(-\frac{16}{9})-5\mathsf{E}(\frac{16}{25}))-2877(5\mathsf{K}(-\frac{16}{9})-3\mathsf{K}(\frac{16}{25}))+15\ln(729))}{256})\\ &\simeq \frac{2}{|\lambda|}0.0188906\end{aligned}$$

where K is the complete elliptic integral of the first kind and E is the complete elliptic integral of the second kind. It might be argued that these integrals were calculated on the semi-axis $\mathbb{R}_+$, while the hermitian product should be calculated on $\mathbb{R}$ and might vanish by symmetry cancellation (in case of odd parity, integrals on $\mathbb{R}_+$ and on $\mathbb{R}_-$ have opposite sign). However, since we have already proved that all anomalous wave functions are either even or odd, then out of the three states (ξ_0, ξ_1, ξ_2), two have necessarily the same parity; thus, the corresponding scalar product is non zero, and these solutions are not orthogonal to each other.

This is a surprising result which requires more insight into the properties of wave functions in quantum mechanics, which we will discuss briefly afterward.

4.2.3. Orthogonality between regular and anomalous solutions Regular and anomalous solutions have different energies so they are expected to be mutually orthogonal as well (see also the discussion afterward).

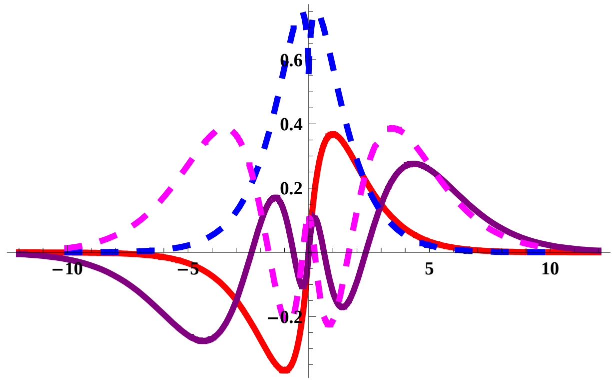

Figure 5. ζ_1 (red, full line), ζ_3 (purple, full line), ξ_0 (blue, dashed line) and ξ_2 (magenta, dashed line).

Performing the hermitian product on the semi-axis $\mathbb{R}_+$ of $\psi(x, E_n) = \zeta_n(\frac{|\lambda|x}{2n})$ with $\psi(x, \tilde{E}_p) = \xi_p(\frac{|\lambda|x}{2p+1})$ yields a non zero result. For instance,

$$\int_0^\infty dx \overline{\psi(x, \tilde{E}_0)}\psi(x, E_1) = \int_0^\infty dx \overline{\xi_0(|\lambda|x)}\zeta_1(\frac{|\lambda|x}{2}) = \frac{2}{3\sqrt{\pi}|\lambda|} \; ;$$

similar expressions can be obtained for all $n \in \mathbb{N}^*$ and $p \in \mathbb{N}$, they can all be written as $r/(q\sqrt{\pi}|\lambda|)$, with integers r and q depending on p and n. Thus, orthogonality between regular and anomalous wave functions can be assured only by *symmetry cancellation* of the right part of the hermitian product (on $\mathbb{R}_+$) with its left part (on $\mathbb{R}_-$).

This leads to the following constraints: first, like the anomalous solutions, all regular solutions must have a definite parity. This is satisfied for $\mu = \pm 1$. Second, all regular solutions must have the same parity, and all anomalous solutions must have the other parity. This means $\mu = \nu$ is fixed. There remains a global choice of sign; either one chooses all regular solutions to be odd and all anomalous solutions to be even or *vice versa*.

While we have no rigorous argument for either case, one notes that the choice $\mu = \nu = 1$ implies that ζ_n, ζ_n' and ξ_n are continuous. This seems to us the natural choice. Consequently, regular solutions ζ_n are odd and anomalous solutions ξ_n are even. The first few solutions are shown in Fig. 5. With this choice, all solutions are continuous at $u = 0$, whereas the first and second derivative of ξ_n are infinite at $u = 0$ (this point is actually a ramification point).

5. Discussion

Despite its apparent simplicity, this one-dimensional problem leads to many interesting results, some of them unexpected. In the following, we will list our main results and discuss some of them.

5.1. Zero transmission through the barrier

The fact that $T = 0$ for a repulsive infinite potential is in agreement with classical mechanics. On the contrary, for an attractive potential, it contradicts classical

mechanics. An example of perfect reflection from an attractive potential, called quantum reflection, is provided by the infinite square well potential:

$$V(x) = V_\mathrm{o} \times \begin{cases} 1 & \text{for } |x| \leq a \ , \\ 0 & \text{for } |x| > a \ , \end{cases} \qquad V_\mathrm{o} \to -\infty \ ,$$

where $2a$ is the width of the well. The Coulomb potential provides us with a new example of pure reflection. It differs from the infinite square well case by the width, which becomes narrower as one goes down in energy, and by the divergence of $\int V(x)dx$, which is logarithmic, while it is faster for the square well potential. Note that both the Coulomb potential and the infinite square well have an infinite number of bound states at negative energy. However, while the spectrum of the former is bounded from below, the spectrum of the latter is not. This is the only example of zero transmission and bounded spectrum that we know of.

As a consequence of $T = 0$, singular unbound wave functions are eventually discarded, but the demonstration is much more involved than in the three-dimensional case of Eq. (2). If one looks back at relations (42a,42b,42c,42d,42e,42f,42g,42h), one finds that all B and b coefficients cancel: the logarithmic solution is completely suppressed, and therefore, the probability density is strictly zero at $x = 0$. In the case of ψ_L, it is zero for $x \geq 0$; in the case of ψ_R, it is zero for $x \leq 0$; the reflection process takes place entirely on the half-line. This suppression at $x = 0$ can be physically interpreted as a hard wall repulsion. It is also true for regular bound states, which probability density cancels at $x = 0$. But it is not the case for anomalous bound states, which show, here again, a special behavior.

5.2. Representation of the S matrix

In one-dimensional scattering problem with symmetric potential $V(x) = V(-x)$, the S matrix is given by Eq. (15). Writing $t = \sqrt{T}\,\mathrm{e}^{\mathbf{i}\theta_t}$ and $r = \sqrt{1-T}\,\mathrm{e}^{\mathbf{i}\theta_r}$, the unitarity of S implies $\cos(\theta_t - \theta_r) = 0$. Therefore, the most general expression of the S matrix can reduce to

$$S = \mathrm{e}^{\mathbf{i}\theta_t} \begin{pmatrix} \epsilon''\sqrt{1-T} & \sqrt{T} \\ \sqrt{T} & \epsilon''\sqrt{1-T} \end{pmatrix} \ , \tag{36}$$

where $0 \leq \theta_t < 2\pi$ and $\epsilon'' = \pm 1$ is an arbitrary sign. The form of Eq. (16) is unique to the Coulomb problem and reduces the number of free parameters, since there is only one continuous parameter T and two arbitrary signs ϵ and ϵ'. In particular, the phase θ_t is now given by

$$\tan(\theta_t) = \frac{\epsilon}{\epsilon'\sqrt{T(1-T}} \ .$$

More precisely, (16) relies on relations (12a), (12b) and on the reflection symmetry of the potential. For any symmetrical potential, one can choose a basis of solutions (f, g) such that (12a) holds; however, any generalization of relation (17a) will fix the ratio A/a or B/b so that (12b) will be changed.

Note that, with $T = 0$, one simply gets $S = -I_2$.

5.3. Non hermiticity of H

The non orthogonality between anomalous bound states implies that H is not perfectly hermitian, because it is well established that the eigenstates of an hermitian operator

are orthogonal. This problem is raised by the same singularity than that, which is calculated in (22b). Indeed, the quantity Δ_{np} defined by

$$\int dx \overline{\xi_n(x\frac{2n+1}{|\lambda|})}\left[-\xi_p''(x\frac{2p+1}{|\lambda|})+\frac{|\lambda|}{|x|}\xi_p(x\frac{2p+1}{|\lambda|})\right]-\int dx\left[-\overline{\xi_n''(x\frac{2n+1}{|\lambda|})}+\frac{|\lambda|}{|x|}\overline{\xi_n(x\frac{2n+1}{|\lambda|})}\right]\xi_p(x\frac{2p+1}{|\lambda|})$$
$$= \lim_{\varepsilon\to 0^+} |\lambda| \left[\frac{\overline{\xi_n(u)}}{2p+1}\frac{d\xi_p}{du}(u) - \overline{\frac{d\xi_n}{du}(u)}\frac{\xi_p(u)}{2n+1}\right]_{-\varepsilon}^{\varepsilon}$$

is not zero, for instance $\Delta_{01} = -\frac{8}{3\pi}$, $\Delta_{02} = \frac{28}{5\pi}$, $\Delta_{03} = -\frac{116}{7\pi}$, $\Delta_{12} = -\frac{4}{5\pi}$, $\Delta_{13} = \frac{23}{7\pi}$, $\Delta_{23} = \frac{27}{14\pi}$, etc.

But the situations are quite different. In the case of the unbound spectrum, eigenstates must be strictly orthogonal; otherwise, a quantum of a given energy E, coming from the frontiers of the universe and interacting with the system would not only create particles of the same energy, but of other energies, so E becomes blurred; but this blurring would spoil into the whole universe, which is impossible. So, we have discarded this possibility (proving therefore $T = 0$) of a break of hermiticity of H.

On the other hand, a bound state of energy E may relax into a coherent state, thanks to interacting overlaps between non orthogonal eigenstates. Thus, it may be excited into a free state of different energy, with a certain probability, which we will examine; yet, this mechanism does not contradict any physical law, and is possible.

Moreover, H is still an observable : its spectrum is *real*, and canonical quantization theory is still valid, so a break of hermiticity restrictedly for $E \in \{\tilde{E}_n, n \in \mathbb{N}\}$ does not yield any contradiction of quantum mechanics, although its exceeds its standard axiomatic formulation.

5.3.1. Coherent bound states Anomalous bound states are not orthogonal, so they are not stable: the spontaneous transition $\tilde{E}_n \to \tilde{T}_p$ is allowed, without any interaction term in the Hamiltonian, which contradicts the standard properties of quantum mechanics. Therefore, a state of energy $\tilde{E}_n$ is not stable. However, the transfer probability between two states of energies $\tilde{E}_n$ and $\tilde{E}_p$ is very small and decreases as $|\tilde{E}_n - \tilde{E}_p|$ is increased, so, anomalous states are almost stable, and their actual energy is only slightly blurred. In order to calculate stable states, one simply needs to diagonalize the (infinite) matrix $M = (\langle\xi_m|\xi_n\rangle)_{m,n}$. M is replaced by truncated matrix $M^{(N)}$, of size $N \times N$ corresponding to $0 \le m, n \le N-1$, and we have diagonalized $M^{(N)}$ instead. By chance, the coefficients of $M^{(N)}$ are rapidly converging when N is increased, so we can calculate numerically those of M.

Let $P^{(N)}$ be the corresponding change of basis matrix. $P^{(N)}$ is indeed close to unity; we show, in Fig. 6 the rapid decrease of $P^{(N)}_{1,N}$ versus N, in Fig. 7 the diagonal coefficient $P^{(N)}_{1,1}$ versus N, and, in Fig. 8 the convergence of $P^{(N)}_{1,q}$ versus N, for some values of q (these coefficients are divided by $P^{(q)}_{1,q}$ for convenience). One verifies that the diagonal coefficient deviation from 1 remains very small, and, correspondingly, that other coefficients are of several orders smaller.

The stable states that we have calculated are coherent states. Each coherent state can be labeled by the closest state of energy $\tilde{E}_n$ and will be written $\tilde{\xi}_n$. When a state of energy $\tilde{E}_n$ is created, it will relax to $\tilde{\xi}_n$. The delay of this relaxation is of the order $\frac{\hbar}{\Delta\tilde{E}_n}$, where $\Delta\tilde{E}_n$ is the uncertainty of $\tilde{E}_n$ due to the instability process and can be explicitly calculated.

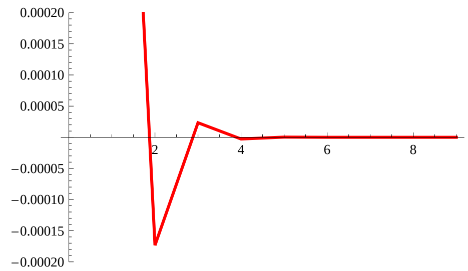

Figure 6. $P_{1,N}^{(N)}$ versus N.

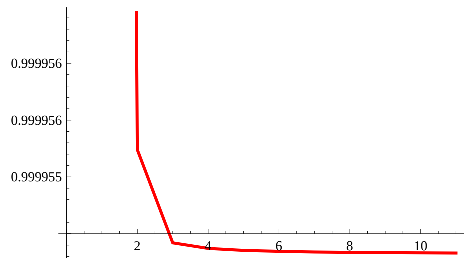

Figure 7. $M_{1,1}^{(N)}$ versus N (it is normalized to 1).

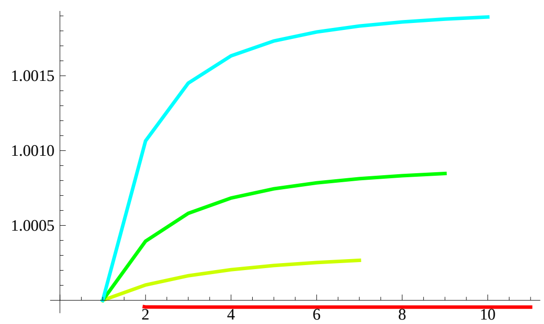

Figure 8. $M_{1,1}^{(N)}$ (red), $M_{1,2}^{(N)}$ (blue), $M_{1,3}^{(N)}$ (green) and $M_{1,5}^{(N)}$ (yellow) versus N (coefficient $P_{1,q}^{(N)}$ is divided by $P_{1,q}^{(q)}$ to show the relative convergence).

On the other hand, consider an excited state of energy $E = -\tilde{E}_p$; even if the state was initially created as ξ_n with $n \neq p$, the probability of exciting state ξ_p, although small, is never zero.

5.3.2. Orthogonality between regular and anomalous states Finally, we would like to insist on the orthogonality between regular and anomalous states. Otherwise, spontaneous relaxation between regular states, $E_n \to E_p$, might occur, through channel $E_n \to \tilde{E}_q \to E_p$, and the effective overlap between regular states would not be zero.

If one adds, in the Hamiltonian, an interaction term between regular and anomalous term, allowing in-between transitions, the exact calculation of transfer probability would become more complicated, because of the relaxation process.

Eventually, in a real system, one should take into account the dynamical aspect of the problem, and consider, instead of a coherent state, an intermediate state, which would include the real dynamical relaxation process. Although it may seem complicated, this opens interecting directions.

6. Conclusion

Simple quantum mechanics can always bring new and surprising results. Indeed, we have found that the hermiticity of the Coulomb Hamiltonian may break exclusively for a closed family of bound states, which we therefore called anomalous states. These states are not stable, and one can only observe, instead, coherent states. We have also found a new case of quantum reflection, by solving the one dimension Coulomb problem.

Acknowledgments
We would like to thank J.-M. Luck and R. Balian for invaluable help and suggestions.

Appendix

A. Asymptotic behavior of F_η and G_η when $u \to -\infty$

Here we analyze the asymptotic behavior of $F_\eta(u)$ and $G_\eta(u)$ for $u \to -\infty$. Our results are different from those in Eqs. (6c) and (6d) in Ref. [1], (see [13]).

Let us first demonstrate (11a). First note that

$$t\,\mathrm{e}^{\mathrm{i}t} M(1+\mathrm{i}\eta, 2, -2\mathrm{i}u) = \overline{t\,\mathrm{e}^{-\mathrm{i}t} M(1-\mathrm{i}\eta, 2, 2\mathrm{i}u)}\ , \tag{36}$$

but, since it is real, one can omit the conjugation. For $u > 0$, writing $u = |u|$ and using (9a), one gets

$$|u|\,\mathrm{e}^{-\mathrm{i}|u|} M(1-\mathrm{i}\eta, 2, 2\mathrm{i}|u|) \underset{|u|\to+\infty}{\sim} \mathrm{e}^{\frac{\pi\eta}{2}} \kappa_\eta \sin(|u| - \Theta_\eta(u))\ .$$

For $u < 0$, writing $u = -|u|$ and using (36), one gets

$$|u|\,\mathrm{e}^{\mathrm{i}|u|} M(1+\mathrm{i}\eta, 2, -2\mathrm{i}|u|) \underset{|u|\to+\infty}{\sim} \mathrm{e}^{\frac{\pi\eta}{2}} \kappa_\eta \underbrace{\sin(|u| - \Theta_\eta(u))}_{=-\sin(u+\Theta_\eta(u))}\ ;$$

if you make $\eta \to -\eta$ in the last relation, and multiply by -1, you get

$$-|u|\,\mathrm{e}^{\mathrm{i}|u|} M(1-\mathrm{i}\eta, 2, -2\mathrm{i}|u|) \underset{|u|\to+\infty}{\sim} \mathrm{e}^{-\frac{\pi\eta}{2}} \kappa_\eta \sin(u - \Theta_\eta(u))\ ,$$

which is exactly the expected relation

$$F_\eta(-|u|) \underset{|u|\to+\infty}{\sim} \mathrm{e}^{-\pi\eta} \sin(u - \Theta_\eta(u))\ .$$

We only write here the leading order of (11a), you must be very careful of all sign compensations for the next orders. Eventually, if one makes again $\eta \to -\eta$ in the last relation, one gets directly

$$F_{-\eta}(-|u|) \underset{|u|\to+\infty}{\sim} \mathrm{e}^{\pi\eta} \sin(u + \Theta_\eta(u))\ ,$$

which is the behavior of $f_\eta(u)$ for $u \sim -\infty$.

The demonstration is very similar, for (11b). First note that

$$t\,\mathrm{e}^{\mathbb{i}t}U(1+\mathbb{i}\eta,2,-2\mathbb{i}u)=\overline{t\,\mathrm{e}^{-\mathbb{i}t}U(1-\mathbb{i}\eta,2,2\mathbb{i}u)}\ ; \tag{37}$$

here, conjugation can not be omitted. For $u>0$, writing $u=|u|$, using (9b) and keeping only the real part, one gets

$$\Re\left(|u|\,\mathrm{e}^{-\mathbb{i}|u|}U(1-\mathbb{i}\eta,2,2\mathbb{i}|u|)\right)\underset{|u|\to+\infty}{\widetilde{\qquad}}\frac{\mathrm{e}^{-\frac{\pi\eta}{2}}}{2\eta\Re(\Gamma(-\mathbb{i}\eta))}\frac{\cos(|u|-\Theta_\eta(u))}{\kappa_\eta}\ .$$

For $u<0$, writing $u=-|u|$, using (37) and still keeping only the real part, one gets

$$\Re\left(|u|\,\mathrm{e}^{\mathbb{i}|u|}U(1+\mathbb{i}\eta,2,-2\mathbb{i}|u|)\right)\underset{|u|\to+\infty}{\widetilde{\qquad}}\frac{\mathrm{e}^{-\frac{\pi\eta}{2}}}{2\eta\Re(\Gamma(\mathbb{i}\eta))}\frac{1}{\kappa_\eta}\underbrace{\cos(|u|-\Theta_\eta(u))}_{=\cos(u+\Theta_\eta(u))}\ .$$

if you make $\eta\to-\eta$ in the last relation, and multiply by -1, you get

$$\Re\left(-|u|\,\mathrm{e}^{\mathbb{i}|u|}U(1-\mathbb{i}\eta,2,-2\mathbb{i}|u|)\right)\underset{|u|\to+\infty}{\widetilde{\qquad}}\frac{\mathrm{e}^{\frac{\pi\eta}{2}}}{2\eta\Re(\Gamma(-\mathbb{i}\eta))}\frac{\cos(u-\Theta_\eta(u))}{\kappa_\eta}\ ,$$

which is exactly

$$G_\eta(-|u|)\underset{|u|\to+\infty}{\widetilde{\qquad}}\mathrm{e}^{\pi\eta}\cos(u-\Theta_\eta(u))\ .$$

Eventually, if one makes again $\eta\to-\eta$ in the last relation, one gets directly

$$G_{-\eta}(-|u|)\underset{|u|\to+\infty}{\widetilde{\qquad}}\mathrm{e}^{-\pi\eta}\cos(u+\Theta_\eta(u))\ ,$$

which is the behavior of $g\eta(u)$ for $u\sim-\infty$.

B. Expression of t as a function of T

First, you get simple relations between (t_α,r_α) and $(A_\alpha,B_\alpha,a_\alpha,b_\alpha)$ (α =R,L) :

$$A_\mathrm{L}=\mathbb{i}t_\mathrm{L}\ ; \tag{38a}$$
$$B_\mathrm{L}=t_\mathrm{L}\ ; \tag{38b}$$
$$a_\mathrm{L}=\mathbb{i}\,\mathrm{e}^{-\pi\eta}(1-r_\mathrm{L})\ ; \tag{38c}$$
$$b_\mathrm{L}=\mathrm{e}^{\pi\eta}(1+r_\mathrm{L})\ ; \tag{38d}$$
$$A_\mathrm{R}=-\mathbb{i}(1-r_\mathrm{R})\ ; \tag{38e}$$
$$B_\mathrm{R}=1+r_\mathrm{R}\ ; \tag{38f}$$
$$a_\mathrm{R}=-\mathbb{i}\,\mathrm{e}^{-\pi\eta}t_\mathrm{R}\ ; \tag{38g}$$
$$b_\mathrm{R}=\mathrm{e}^{\pi\eta}t_\mathrm{R}\ . \tag{38h}$$

The unitarity of S writes

$$|r|^2+|t|^2=1\ ; \tag{39a}$$
$$\bar{t}r+r\bar{t}\quad=0\ . \tag{39b}$$

From (39b) one deduce

$$\frac{t}{|t|}=\mathbb{i}\epsilon\frac{r}{|r|}\ , \tag{40}$$

where $\epsilon = \pm 1$. From relations (38b,38d), one gets

$$\frac{b_{\mathrm{L}}\,\mathrm{e}^{-\pi\eta}}{B_{\mathrm{L}}} = \frac{1+r}{t}\ .$$

By use of relations (39a,39b), this writes

$$\frac{b_{\mathrm{L}}\,\mathrm{e}^{-\pi\eta}}{B_{\mathrm{L}}} = \frac{1+\mathbb{i}\epsilon t\sqrt{\frac{1-T}{T}}}{t}\ ,$$

but Eq. (17a) implies the existence of $\theta \in \mathbb{R}$ such that

$$\frac{b_{\mathrm{L}}\,\mathrm{e}^{-\pi\eta}}{B_{\mathrm{L}}} = \mathrm{e}^{\mathbb{i}\theta}\ ,$$

so, using back relation (14), we get

$$\frac{1}{t} = \mathrm{e}^{\mathbb{i}\theta} - \mathbb{i}\epsilon\sqrt{\frac{1}{|t|^2}-1}\ .$$

We carefully multiply this equation by its conjugate and find

$$\frac{1}{|t|^2} = 1 + \frac{1}{|t|^2} - 1 - 2\epsilon\sin(\theta)\sqrt{\frac{1}{|t|^2}-1}\ ,$$

which implies $\theta = 0$ or π. We will write $\mathrm{e}^{\mathbb{i}\theta} = \epsilon'$ then

$$\frac{1}{t} - \epsilon' = -\mathbb{i}\epsilon\sqrt{\frac{1}{|t|^2}-1}\ .$$

We carefully multiply this equation by its conjugate and find

$$\frac{1}{|t|^2} + 1 - \epsilon'\frac{2\Re(t)}{|t|^2} = \frac{1}{|t|^2} - 1 \iff \Re(t) = \epsilon'|t|^2\ ,$$

but $|t|^2 = \Re(t)^2 + \Im(t)^2$, so we get

$$|t|^2 = |t|^4 + \Im(t)^2 \iff \Im(t) = \epsilon''\sqrt{|t|^2-|t|^4}\ .$$

By use of (14), we have $t = \Re(t) + \mathbb{i}\Im(t) = \epsilon' T + \mathbb{i}\epsilon''\sqrt{T-T^2}$. We eventually shall prove that $\epsilon'' = \epsilon$. We put the last expression of t into $(1+r)/t$ and get

$$\begin{aligned}\frac{1+r}{t} &= \frac{1+\mathbb{i}\epsilon t\sqrt{\frac{1}{T}-1}}{t} = \frac{(1-\epsilon\epsilon''+T\epsilon(\epsilon''+\mathbb{i}\epsilon'\sqrt{\frac{1}{T}-1}))(\epsilon' T - \mathbb{i}\epsilon''\sqrt{T-T^2})}{T}\\ &= \epsilon' + \mathbb{i}(\epsilon-\epsilon'')\sqrt{\frac{1}{T}-1}\ .\end{aligned}$$

By taking the modulus of this expression, you would find indeed that $\epsilon = \epsilon''$. However, we already know that it is real (because $\theta = 0$ or π), so you have the result straight. Now, if you use back the different relations, you can get the final expression of T :

$$t = \epsilon' T + \mathbb{i}\epsilon\sqrt{T(1-T)} \tag{41}$$

where $\epsilon' = \pm 1$ is independent of ϵ. By use of relations (38e,38f,38g,38h,38a,38b,38c,38d), (41) and (17a), after some calculations, one gets

$$\begin{aligned}
A_{\rm L} &= -\epsilon\sqrt{T(1-T)} + \mathbb{i}\epsilon' T \ ; && (42a)\\
B_{\rm L} &= \epsilon' T + \mathbb{i}\epsilon\sqrt{T(1-T)} \ ; && (42b)\\
a_{\rm L} &= \mathrm{e}^{-\pi\eta}(\epsilon\epsilon'\sqrt{T(1-T)} + \mathbb{i}(2-T)) \ ; && (42c)\\
b_{\rm L} &= \mathrm{e}^{\pi\eta}(T + \mathbb{i}\epsilon\epsilon'\sqrt{T(1-T)}) \ ; && (42d)\\
A_{\rm R} &= -\epsilon\epsilon'\sqrt{T(1-T)} - \mathbb{i}(2-T) \ ; && (42e)\\
B_{\rm R} &= T + \mathbb{i}\epsilon\epsilon'\sqrt{T(1-T)} \ ; && (42f)\\
a_{\rm R} &= \mathrm{e}^{-\pi\eta}(\epsilon\sqrt{T(1-T)} - \mathbb{i}\epsilon' T) \ ; && (42g)\\
b_{\rm R} &= \mathrm{e}^{\pi\eta}(\epsilon' T + \mathbb{i}\epsilon\sqrt{T(1-T)}) \ ; && (42h)
\end{aligned}$$

and

$$r = T - 1 + \mathbb{i}\epsilon\epsilon'\sqrt{T(1-T)} \ . \qquad (42i)$$

Using these relations, one verifies all relations (14,39a,39b) and (17b).

An important collateral result from this demonstration is indeed that

$$\frac{b_{\rm L}\,\mathrm{e}^{-\pi\eta}}{B_{\rm L}} = \epsilon' \ ;$$

from relations (38f,38b,38h,38d), one gets

$$\frac{b_{\rm R}\,\mathrm{e}^{-\pi\eta}}{B_{\rm R}} = \frac{b_{\rm L}\,\mathrm{e}^{-\pi\eta}}{B_{\rm L}} = \epsilon'$$

which proves, by linearity, relation (17b).

C. Mclaurin expansions

Here we study the behavior of basic solutions $f_\eta(u)$, $g_\eta(u)$ and their derivatives when $u \to 0$. Let us consider first the expansion of F_η and G_η for $u \to 0^+$, which are given by[10] :

$$\begin{aligned}
F_\eta(u) &\simeq \mathrm{e}^{-\frac{\pi\eta}{2}}|\Gamma(1+\mathbb{i}\eta)|(u+\eta t^2)\\
&= C_\eta(u+\eta t^2)\\
G_\eta(u) &\simeq \frac{1}{C_\eta}\left\{2\eta(u+\eta u^2)\Big(\log(2u) - 1 + p(\eta) + 2\gamma_{\rm E}\Big) + (1 - \frac{1+6\eta^2}{2}u^2)\right\}
\end{aligned}$$

$$\begin{aligned}
\frac{dF_\eta}{du}(u) &\simeq C_\eta(1+2\eta u)\\
\frac{dG_\eta}{du}(u) &\simeq \frac{1}{C_\eta}\left\{2\eta\left[(1+2\eta u)\Big(\log(2u) + p(\eta) + 2\gamma_{\rm E}\Big) - \eta u\right] - (1+6\eta^2)u\right\}
\end{aligned}$$

$$\begin{aligned}
\frac{d^2F_\eta}{du^2}(u) &\simeq C_\eta 2\eta\\
\frac{d^2G_\eta}{du^2}(u) &\simeq \frac{1}{C_\eta}\left\{2\eta\left[2\eta\Big(\log(2u) + p(\eta) + 2\gamma_{\rm E}\Big) + \eta + \frac{1}{u}\right] - (1+6\eta^2)\right\}
\end{aligned}$$

with $p(\eta) = \Re\left(\frac{\Gamma'(1+\mathbf{i}\eta)}{\Gamma(1+\mathbf{i}\eta)}\right) = p(-\eta)$ and γ_{E} is Euler's constant. Thus, one gets, at first order, for the complete solution φ,

$$\varphi(u,\eta) \underset{u\to 0^+}{\widetilde{\quad}} B\frac{1}{C_\eta} \; ; \tag{43a}$$

$$\varphi(u,\eta) \underset{u\to 0^-}{\widetilde{\quad}} b\frac{\mathrm{e}^{-\pi\eta}}{c_\eta} = \frac{b}{C_{-\eta}} \; ; \tag{43b}$$

$$\frac{\partial\varphi}{\partial u}(u,\eta) \underset{u\to 0^+}{\widetilde{\quad}} AC_{-\eta} + 2B\eta\frac{1}{C_{-\eta}}(\log(2u) + p(\eta) + 2\gamma_{\mathrm{E}}) \; ; \tag{43c}$$

$$\frac{\partial\varphi}{\partial u}(u,\eta) \underset{u\to 0^-}{\widetilde{\quad}} aC_{-\eta} - 2b\eta\frac{1}{C_{-\eta}}(\log(-2u) + p(\eta) + 2\gamma_{\mathrm{E}}) \; . \tag{43d}$$

D. Orthonormality relations

The purpose of this section is to calculate the limit, when $L \to \infty$ of $\int_{-L}^{L} \overline{\psi(x,E_1,\alpha_1)}\psi(x,E_2,\alpha_2)dx$. Consider a given L, this integral with all functions replaced by their asymptote (12a) or (12b) becomes:

$$\begin{aligned}
\frac{1}{2}\int_0^L \; & dx \cos\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}} + \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) - \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) A^+_{\alpha_1\alpha_2} \\
& - \cos\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}} - \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) - \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) A^-_{\alpha_1\alpha_2} \\
& + \sin\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}} - \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) - \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) B^+_{\alpha_1\alpha_2} \\
& + \sin\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}} + \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) - \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) B^-_{\alpha_1\alpha_2} \\
+\frac{1}{2}\int_{-L}^0 & dx \cos\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}} - \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) + \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) a^+_{\alpha_1\alpha_2} \\
& - \cos\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}} + \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) + \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) a^-_{\alpha_1\alpha_2} \\
& + \sin\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}} + \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) + \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) b^+_{\alpha_1\alpha_2} \\
& + \sin\left(\frac{\lambda x}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}} - \Theta_{\eta_1}(\frac{x\lambda}{2\eta_1}) + \Theta_{\eta_2}(\frac{x\lambda}{2\eta_2})\right) b^-_{\alpha_1\alpha_2}
\end{aligned}$$

where we use

$$\begin{aligned}
A^+_{\alpha_1\alpha_2} &= (\overline{A_{\alpha_1}}A_{\alpha_2} + \overline{B_{\alpha_1}}B_{\alpha_2}) \; ; \qquad & A^-_{\alpha_1\alpha_2} &= (\overline{A_{\alpha_1}}A_{\alpha_2} - \overline{B_{\alpha_1}}B_{\alpha_2}) \; ; \\
B^+_{\alpha_1\alpha_2} &= (\overline{A_{\alpha_1}}B_{\alpha_2} + \overline{B_{\alpha_1}}A_{\alpha_2}) \; ; \qquad & B^-_{\alpha_1\alpha_2} &= (\overline{A_{\alpha_1}}B_{\alpha_2} - \overline{B_{\alpha_1}}A_{\alpha_2}) \; ; \\
a^+_{\alpha_1\alpha_2} &= \overline{a_{\alpha_1}}a_{\alpha_2}\,\mathrm{e}^{\pi(\eta_1+\eta_2)} + \overline{b_{\alpha_1}}b_{\alpha_2}\,\mathrm{e}^{-\pi(\eta_1+\eta_2)}) \; ; \\
a^-_{\alpha_1\alpha_2} &= \overline{a_{\alpha_1}}a_{\alpha_2}\,\mathrm{e}^{\pi(\eta_1+\eta_2)} - \overline{b_{\alpha_1}}b_{\alpha_2}\,\mathrm{e}^{-\pi(\eta_1+\eta_2)}) \; ; \\
b^+_{\alpha_1\alpha_2} &= \overline{a_{\alpha_1}}b_{\alpha_2}\,\mathrm{e}^{\pi(\eta_1-\eta_2)} + \overline{b_{\alpha_1}}a_{\alpha_2}\,\mathrm{e}^{-\pi(\eta_1-\eta_2)}) \; ; \\
b^-_{\alpha_1\alpha_2} &= \overline{a_{\alpha_1}}b_{\alpha_2}\,\mathrm{e}^{\pi(\eta_1-\eta_2)} - \overline{b_{\alpha_1}}a_{\alpha_2}\,\mathrm{e}^{-\pi(\eta_1-\eta_2)}) \; .
\end{aligned}$$

The difference with the exact limit is finite and contributes to constant c in formula (19). Now, these integrations are easily performed when one notes that all $\Theta_\eta(u)$ functions can be treated as constant. Indeed, let us consider a simpler integral $\int_0^L \cos(su+\ln(u))du$, where we will omit the problem at $u=0$, and $\delta(L)\equiv \frac{1}{s}\sin(su+\ln(u))-\int_0^L\cos(su+\ln(u))du$ is the difference of the approximate integral with the exact one. Then, $\delta'(L)=\frac{\sin(sL+\ln(L))}{sL}$ not only tends to zero when $L\to\infty$, but has a finite integral $\int_0^L\delta'(u)du$. This proves that all such approximations are valid and simply contribute to constant c.

The $x=0$ boundary only contributes to constant c (you may need to replace $x=0$ with another boundary, in order to avoid any divergence, but this replacement simply gives another contribution to constant c) so we may skip it and eventually get

$$
\begin{aligned}
\frac{1}{\lambda}\Bigg[&\frac{\eta_1\eta_2}{\eta_1-\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)A^+_{\alpha_1\alpha_2}\\
&+\frac{\eta_1\eta_2}{\eta_1+\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)A^-_{\alpha_1\alpha_2}\\
&-\frac{\eta_1\eta_2}{\eta_1+\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)B^+_{\alpha_1\alpha_2}\\
&-\frac{\eta_1\eta_2}{\eta_1-\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)B^-_{\alpha_1\alpha_2}\\
&-\frac{\eta_1\eta_2}{\eta_1-\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)a^+_{\alpha_1\alpha_2}\\
&+\frac{\eta_1\eta_2}{\eta_1+\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)a^-_{\alpha_1\alpha_2}\\
&+\frac{\eta_1\eta_2}{\eta_1+\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)b^+_{\alpha_1\alpha_2}\\
&+\frac{\eta_1\eta_2}{\eta_1-\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)b^-_{\alpha_1\alpha_2}\Bigg].
\end{aligned}
$$

Now, both limits of $\frac{\sin(sL)}{s}$ and $\frac{\cos(sL)}{s}$ when $L\to\infty$ are equal to $\pi\delta(s)$ (with differential ds). The $\ln(u)$ correction has no influence (see Appendix E). Then we write $\delta(\frac{1}{\eta_2}-\frac{1}{\eta_1})=\delta(\frac{2}{\lambda}(k_1-k_2))=\frac{\lambda}{2}\delta(k_1-k_2)$, so we eventually get factor $\frac{\pi}{\lambda}\frac{\lambda}{2}$. We have forgotten the exact differential $\frac{dk}{2\pi}$ in one dimension, and we will include a last factor 2 which accounts for the equality between the limits of $\int_0^L$ and $\int_{-L}^0$. Altogether, we get formula (19), with the following coefficients of matrix P :

$$
P_{\alpha\alpha'}=\frac{\overline{A_\alpha}A_{\alpha'}+\overline{B_\alpha}B_{\alpha'}+\overline{a_\alpha}a_{\alpha'}\,\mathrm{e}^{2\pi\eta}+\overline{b_\alpha}b_{\alpha'}\,\mathrm{e}^{-2\pi\eta}}{2}
$$

and, with relations (42e,42f,42g,42h,42a,42b,42c,42d), we eventually get

$$
P=\begin{pmatrix}1&0\\0&1\end{pmatrix},
$$

thus (18) is verified.

E. Hermiticity relations at infinity

The calculation of (22a) is similar to the previous orthonormality calculations, although simpler. Here $\alpha = R, L$ for the choice of φ_α and we use the notations of Appendix D. One gets

$$\begin{aligned}
&\frac{\eta_1+\eta_2}{2\eta_1\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)A^+_{\alpha\alpha}\\
&-\frac{\eta_1-\eta_2}{2\eta_1\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)A^-_{\alpha\alpha}\\
&-\frac{\eta_1-\eta_2}{2\eta_1\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)B^+_{\alpha\alpha}\\
&+\frac{\eta_1+\eta_2}{2\eta_1\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})-\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)B^-_{\alpha\alpha}\\
&-\frac{\eta_1+\eta_2}{2\eta_1\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)a^+_{\alpha\alpha}\\
&+\frac{\eta_1-\eta_2}{2\eta_1\eta_2}\sin\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)a^-_{\alpha\alpha}\\
&+\frac{\eta_1-\eta_2}{2\eta_1\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1+\eta_2}}+\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)b^+_{\alpha\alpha}\\
&-\frac{\eta_1-\eta_2}{2\eta_1\eta_2}\cos\left(\frac{\lambda L}{2\frac{\eta_1\eta_2}{\eta_1-\eta_2}}-\Theta_{\eta_1}(\frac{L\lambda}{2\eta_1})+\Theta_{\eta_2}(\frac{L\lambda}{2\eta_2})\right)b^-_{\alpha\alpha}\ .
\end{aligned}$$

One striking thing is that the coefficients $\frac{1}{\eta_1}\pm\frac{1}{\eta_2}$ are very different from the previous case. In order to match with the δ limit, one must divide by $\frac{1}{\eta_1}\mp\frac{1}{\eta_2}$, so there is a global supplementary factor $\frac{1}{\eta_1}^2-\frac{1}{\eta_2}^2$, which, when multiplied by $\delta(\frac{1}{\eta_1}\pm\frac{1}{\eta_2})$, will always give zero.

Another important difference is that we have made no approximation in this case. It is worth studying the last limit more carefully, than we did before. Using again a simpler case, we want to prove that $\lim_{L\to\infty}\frac{1}{s}\sin(sL-s\ln(L)-\kappa s^2+\beta)$ is $\pi\delta(s)$ (κ and β are just constants here). The important thing is that $\tilde{L}\equiv L-\ln(L)\to\infty$ and can be used as a parameter, so the result is proved, and the limit of (22a) is strictly zero.

F. Digression: To WKB or not to WKB?

In a nuclear fission process, a light nucleus of mass m and charge $q=Zq_e>0$ (e.g an alpha particle with $Z=2$) is trapped in a metastable state at energy E due to a potential "pocket" $V(r)=V_N(r)+V_C(r)$ of an heavy nucleus of charge $q'=Z'q_e$ (here r is the distance between the centers of mass of the two nuclei). The potential is the sum of a strong short-range attractive nuclear potential $V_N(r)$ and a repulsive long range Coulomb potential $V_C(r)=\frac{qq'}{r}$. The focus of interest is on the escape probability P from the metastable state. In a crude approximation, $V(r)$ is replaced

by a deep potential well of range R and depth $-V_0$ and a Coulomb tail for $r > R$, see figure 9:

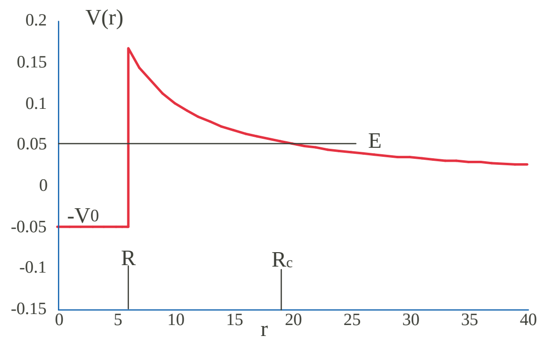

Figure 9. Approximated potential $V(r) = V_N(r) + V_C(r)$ designed to calculate the fission probability within the WKB approximation.

The escape probability is then calculated in the WKB approximation, integrating the local momentum $\kappa(r) = \sqrt{\frac{2m}{\hbar^2}[V_C(r) - E)]}$ between the turning points R and R_c (such that $V_C(R_c) = E$).

$$\Lambda = \int_R^{R_c} \kappa(r)dr = \int_0^{R_c} \kappa(r)dr - \int_0^R \kappa(r)dr \equiv \Lambda_G - \Lambda_R \; ; \qquad P = e^{-2\Lambda} \; .$$

When $R \ll R_c$ the result is written as,

$$P = e^{-\frac{2\pi mqq'}{\hbar v}} e^{\frac{32mqq'R}{\hbar^2}} \equiv P_G T_R, \tag{44}$$

where v is the relative velocity and P_G is the *Gamow factor*, which contains the energy dependence of the escape probability. Relation (27), with $\varepsilon = R$, gives the *exact* escape amplitude $= |t|^2$ (for the special case $V_0 = 0$ but that can be easily modified). It also shows that the WKB expression (44) cannot be used as $R \to 0$ because it yields a finite escape probability while the exact result (within the naive model of figure 9) gives zero escape probability. The reason is that the conditions for the use of the WKB approximation are not met, strictly speaking.

G. Generalization of recurrence equations

We study the changes of relations (14.1) in Ref. [10] for the bound states ($e < 0$), in the case $L = 0$. Note first that (14.1.1) is also changed, it writes now as (29a).

Relation (14.1.6) writes now (we omit the $L = 0$ exponent)

$$A_1 = 1 \; ; \qquad A_2 = \eta \; ; \qquad (k+1)(k+2)A_{k+2} = 2\eta A_{k+1} + A_k \; .$$

Relation (14.1.14) writes now (with our notations)

$$L_\eta(u) = 2\eta K_\eta(u)(\log(2u) - 1 + \frac{\Gamma'(1+\eta)}{\Gamma(1+\eta)} + 2\gamma_{\mathrm{E}}) + \theta_\eta(u)$$

with (14.1.17) (relation (14.1.15) is useless here)

$$\theta_\eta(u) = \sum_{k=0}^{\infty} a_k u^k$$

and relations (14.1.18) to (14.1.20) now become

$$a_0 = 1 \ ; \quad a_1 = -1 \ ; \quad (k+1)(k+2)a_{k+2} = 2\eta a_{k+1} + a_k - 2\eta(2k+3)A_{k+2} \ .$$

Eventually, note that new relation (14.1.14) also holds for $u < 0$ as soon as you replace $\log(2u)$ by $\log(-2u)$.

H. Identities between confluent hypergeometric functions an modified Bessel ones

We found useful identities between confluent hypergeometric functions $M(\frac{1}{2} \pm n, 2, 2t)$ or $U(\frac{1}{2} \pm n, 2, 2t)$ and modified Bessel functions $\mathbf{I}_n(t)$ or $\mathbf{K}_n(t)$, for all $n \in \mathbb{N}$.

These identities appear to generalize some identity established only for $n = 0$ or $n = 1$; indeed, from relations (13.6.3) and (13.6.21) of Ref. [10], one shows

$$\mathrm{e}^{-t} M(\frac{1}{2}, 2, 2t) = \mathbf{I}_0(t) - \mathbf{I}_1(t) \ ; \tag{45a}$$

$$\mathrm{e}^{-t} U(\frac{1}{2}, 2, 2t) \ = \frac{1}{2\sqrt{\pi}}(\mathbf{K}_0(t) + \mathbf{K}_1(t)) \ ; \tag{45b}$$

Thus, it seems possible to generalize this relations and look for solutions of Eqs. (29a) and (29b) in the form

$$f_n(t) = t\Big(p_n(t)\mathbf{I}_0(t) - q_n(t)\mathbf{I}_1(t)\Big) \tag{46a}$$

or

$$g_n(t) = t\Big(p_n(t)\mathbf{K}_0(t) + q_n(t)\mathbf{K}_1(t)\Big) \tag{46b}$$

(we took advantage of further relations between the polynomials (p_n, q_n) defined in Eq. (46a) and those defined in Eq. (46b) in order to save notations.)

Although it works well, it proved more efficient to find directly the recurrence relations which define p_n and q_n. Using relation (13.4.11) of Ref. [10] for $M(\frac{1}{2}-n, 2, 2t)$, (13.4.10) for $M(\frac{1}{2}+n, 2, 2t)$, (13.4.26) for $U(\frac{1}{2}-n, 2, 2t)$ or (13.4.23) for $U(\frac{1}{2}+n, 2, 2t)$, and making the derivative of Eqs. (46a) and (46b) using $\mathbf{I}_0' = \mathbf{I}_1$, $\mathbf{I}_1'(t) = \mathbf{I}_0(t) - \mathbf{I}_1(t)/t$, $\mathbf{K}_0' = -\mathbf{K}_1$ and $\mathbf{K}_1'(t) = -\mathbf{K}_0(t) - \mathbf{K}_1(t)/t$, and fixing $p_0 = q_0 = 1$, one finds, up to some normalisation factors,

$$p_{n+1}(x) = (2n+3)p_n(x) + 2x(p_n'(x) - p_n(x) - q_n(x)) \tag{47a}$$

$$q_{n+1}(x) = (2n+1)q_n(x) + 2x(q_n'(x) - p_n(x) - q_n(x)) \tag{47b}$$

These definitions have one main advantage : these polynomials are real and have integer coefficients ; let us write $p_n(x) = \sum_{i=0}^n a_i^n x^i$ and $q_n(x) = \sum_{i=0}^n b_i^n x^i$, we get $a_0^n = (2n+1)!!$, $b_0^n = (2n-1)!!$, $a_n^n = b_n^n = (-4)^n$.

Eventually, let us fix the normalisation problem (note the symmetry between $M(\frac{1}{2}-n, 2, 2t)$ and $M(\frac{3}{2}+n, 2, 2t)$ or between $U(\frac{1}{2}-n, 2, 2t)$ and $U(\frac{3}{2}+n, 2, 2t)$ and that $(-1)!! = 1$): $\forall n \in \mathbb{N}$,

$$\mathrm{e}^{-t} M(\frac{1}{2} - n, 2, 2t) = \frac{1}{(2n+1)!!}\big(p_n(t)I_0(t) - q_n(t)I_1(t)\big) \ ; \tag{48a}$$

$$\mathrm{e}^{-t} U(\frac{1}{2} - n, 2, 2t) \ = \frac{(-1)^n}{2^{n+1}\sqrt{\pi}}\Big(p_n(t)K_0(t) + q_n(t)K_1(t)\Big) \ ; \tag{48b}$$

$$\mathrm{e}^{-t} M(\frac{3}{2} + n, 2, 2t) = \frac{1}{(2n+1)!!}\big(p_n(-t)I_0(t) + q_n(-t)I_1(t)\big) \ ; \tag{48c}$$

$$\mathrm{e}^{-t} U(\frac{3}{2} + n, 2, 2t) \ = \frac{2^n}{(2n+1)!!(2n-1)!!\sqrt{\pi}}\Big(-p_n(-t)K_0(t) + \ q_n(-t)K_1(t)\Big). \tag{48d}$$

[1] V. S. Mineev, Theor. Math. Phys. **140** 1157 (2004).
[2] F. L. Yost, J. A. Wheelrer & G. Breit, Phys. Rev. **49** 174 (1936).
[3] M. Moshinsky, J. Phys. A **26** 2445 (1993).
[4] J. Basdevant & J. Dalibard, "Quantum Mechanics", Advanced texts in Physics, ed. Springer-Verlag, Berlin Heidelberg (2002).
[5] R. Shankar, "Principles of Quantum Mechanics", ed. Plenum Press, New York (1994).
[6] This is a new boundary condition, not present in the one-dimensional problem., in : D. Bohm, "Quantum Theory", Prentice-Hall Physics series, ed. D. H. Menzel, New york (1951), p. 335.
[7] Y. Takana & S. Kashiwaya, Phys. Rev. Lett **74** 3451 (1995).
[8] E. H. Lieb & W. Liniger, Phys. Rev. **130** 1605 (1963).
[9] It is not clear why the analytic continuation avoiding zero did not give all solutions.
[10] M. Abramowitz & I. A. Stegun, *Handbook of Mathematical Functions*, ed. Dover, New York (1965).
[11] Note that relation (13.1.3) in [10] fails here so one should use instead (13.1.6).
[12] The origin of this we did not elucidate.
[13] We believe there is a mistake in the analysis in § after relation (A18) of Ref. [1].
[14] E. Merzbacher, *Quantum Mechanics*, 2^{nd} ed. J. Wiley, New York (1970).
[15] Y. Imry, *Introduction to Mesoscopic Physics*, ed. Oxford University Press, New York (1997); A somewhat different parametrization is suggested in Y. Avishai & Y. B. Band, Phys. Rev. B **32** 2674 (1985).
[16] The representation of (15) (matrix S), (19) (orthogonality constraints) and (21) (hermiticity constraints) in terms of coefficients $T(\eta)$ are peculiar for the Coulomb problem discussed here, and not valid for any one-dimensional scattering problem.
[17] The essential Coulomb properties are implicitly contained in these relations.
[18] More precisely, $\delta(k_1 + k_2)$ only contribute to $\psi(x, 0)$, which is not an important matter here. It is however interesting to note that the complete weight of this state, within $T = 0$, is found to be zero, which is exact.
[19] Y. Avishai and J. M. Luck, Phys. Rev. B **45**, 1074 (1992).
[20] Mineev claims that it had been already solved many times, but gives no references, except of Ref. [3], which gives not many details.